01 SOLID FUELS

Sources, winning, properties

10/00001 Effect of processing temperature on the bitumen/MDI-PEG reactivity

Martín-Alfonso, M. J. *et al. Fuel Processing Technology*, 2009, 90, (4), 525–530.

Reactive polymers are lately gaining acceptance to give added value to a residue of the crude oil refining process such as bitumen. The resulting material should display enhanced mechanical properties to be considered for advanced applications in construction. This study reports the effect of processing temperature on the reaction between bitumen compounds and an isocyanate-based reactive polymer, synthesized by reaction of polymeric MDI (4,4′-diphenylmethane diisocyanate) with a low molecular weight polyethylene-glycol (PEG). Rheokinetics experiments, viscosity measurements at 60 °C, atomic force microscopy (AFM) characterization, thin layer chromatography (TLC-FID) analysis and thermogravimetric studies (TGA) were performed on the reactive polymer and on samples of MDI-PEG modified bitumen containing 2 wt% of the polymer. Results showed the existence of an optimum processing temperature arisen as a consequence of opposite effects: microstructural availability for the formation of a polymer–bitumen network, reaction ability and polymer thermal degradation. Consequently, this study aims to serve as a guideline for the refining and asphalt industries facing the stage of selecting the optimum processing parameters.

10/00002 Estimations of Clarkes for Carbonaceous biolithes: world averages for trace element contents in black shales and coals

Ketris, M. P. and Yudovich, J. E. *International Journal of Coal Geology*, 2009, 78, (2), 135–148.

Black shale and coal Clarke values are the average trace element contents in the World black shales and coals. These calculations are made in Russian geochemistry but up to now are poorly known in the West. Modern tables of black shale and coal Clarkes are presented, based on comprehensive calculations using very large amount of information (thousands analyses of black shales, coals, and coal ashes for trace elements). In black shale geochemistry, three figures were calculated for each main lithologies: terrigenous (+ uff), chert, and carbonate. Two Clarke estimations are presented, named 'lithological' (K_1) and 'lithostratigraphical' (K_2). In coal geochemistry, seven figures were calculated for each trace element: average content in hard coals and their ashes; average content in brown coals and their ashes; average content in all coals and their ashes; and coal affinity index (or 'coalphile index') = average content in all ashes/Clarke values of sedimentary rocks. The black shale and coal Clarkes presented here provide an important scientific base for many geochemical comparisons and issues.

10/00003 Isotopic composition of lead in Czech coals

Mihaljevič, M. *et al. International Journal of Coal Geology*, 2009, 78, (1), 38–46.

The content and isotopic compositions of lead (Pb) were studied on selected coal samples from the Czech Republic. Simultaneously, the forms of bonding of Pb in coal were studied using sequential extraction (1M ammonium acetate, 3 M HCl, 48% HF and 2 M HNO_3). Lead in most samples of bituminous and brown coal is mobilized by 3 M HCl, while sulfides are already oxidized in the studied samples at the beginning of the extraction (1 M ammonium acetate). Thus, Pb could be bonded in carbonates and oxides and also to sulfides present in the coal. Following decomposition of the sulfides, Pb is adsorbed on the remainder of the solid phase and is released only in the acidic medium of the second extraction solution (i.e. 3 M HCl). Bituminous coal contains an average of 33 mg/kg Pb, while brown coal contains an average of 8.9 mg/kg Pb. The $^{206}Pb/^{207}Pb$ ratio varies in the range 1.167–1.234 for bituminous and 1.172–1.24 for brown coal. No inverse proportionality of the Pb content and the $^{206}Pb/^{207}Pb$ ratio was observed in the studied samples and, thus, the Pb content in most samples is a result of the combination of lithogenic and ore Pb. Only several samples with high uranium contents exhibited a highly radiogenic $^{206}Pb/^{207}Pb$ ratio (>1.3). It was not possible to demonstrate any statistical dependence between the operational defined speciation of Pb, the mineralogical composition and the Pb isotopic composition.

10/00004 Modelling the mechanical thermal expression behaviour of lignite

Wheeler, R. A. *et al. Fuel*, 2009, 88, (9), 1741–1751.

A process known as mechanical thermal expression (MTE) is used to dewater lignite to improve its heating value. A numerical model is developed to investigate the compression dewatering stage of the MTE process at ambient (20 °C) and elevated temperature (150 °C). This model includes details not previously investigated such as the wall friction, the compressive yield stress of the lignite network as a function of void ratio, and the relationship between the yield stress and the absolute permeability. This allows gradients of these properties to develop as dewatering progresses. The results from the model are compared with the void ratio, hydraulic pressure drop and permeability, which are independently determined experimentally. A major simplification in this work is that only primary consolidation is incorporated in the model. The results clearly show that secondary consolidation does occur in lignite, but it is not significant except at low applied pressures, or for compression times which are much longer than would be of industrial interest.

10/00005 Trace elements geochemistry of the Dobrudza coal basin, Bulgaria

Eskenazy, G. M. *International Journal of Coal Geology*, 2009, 78, (3), 192–200.

The paper discusses trace elements in the Dobrudza coal deposit. The deposit is the deepest in Bulgaria. The coal rank reaches the stage of high volatile A bituminous coal. The contents of Ba, Cl, Br, Mn, Ge, Pb, W, Mo, As, Zr, Li, Cs, Cu, Zn, Sb, Ti, V, Th, U, Ag, Be and Y are enriched from 1.5 to 9.2 times as compared with the Clarkes for bituminous coals. The content of the other elements are slightly higher/lower than the respective world-wide means. Chondrite-normalized patterns of the REE reveal a strong fractionation among the HREE and LREE, most pronounced for the coals than for the coaly shales and partings. A specific feature is the small Eu anomaly in the shales and the tonsteins underlying the coal bed. Most elements are of mixed, organic and inorganic association. Ge, Cl, Br, Mo, Be and Au are predominantly bound to the organic matter. Arsenic correlates strongly with Fe suggesting presence in pyrite. Ba occurs mainly as barite which is most probably of epigenetic origin. Sr and Mn are presented mainly as isomorphous admixtures in barite and calcite. The abundance of the lithophile elements (excluding Ge, Mo, Ba, Cl, Br) is controlled largely by the detrital and clay mineral content of the coals. Many elements of different groups correlate positively each other. Calculation of partial correlation coefficients excluding ash shows that many of these correlations are spurious, due to the positive correlation of every single element with ash. For this reason, the correlation coefficients must be critically evaluated when deducing the mode of occurrence of elements. The accumulation of the trace elements in the Dobrudza coals was influenced by multi-component geological factors: (1) Upper Pennsylvanian volcanism, there are widespread tonsteins, underlying the coal layers and as thin layers in the coal. Most likely, many elements were leached from the tonsteins and trapped by the coal. (2) Olivinobasalt and andesito-basalt dikes intruding the coal-bearing sediments may cause enrichment or depletion of many elements. (3) Highly mineralized underground waters are the source of Cl, Br, B, Sr and probably some other elements. (4) The numerous regional faults favour the penetration of solutions of different origin which were carriers of trace elements. (5) Postgenetic erosive processes may cause leaching of trace elements from the rocks which are consequently fixed by the coal.

Preparation

10/00006 Alkali-assisted coal extraction with polar aprotic solvents

Makgato, M. H. *et al. Fuel Processing Technology*, 2009, 90, (4), 591–598.

Coal extraction experiments were conducted using a coal, containing approximately 10% ash, from the Tshikondeni mine in South Africa. This coal dissolves only to a limited extent in pure polar aprotic solvents such as dimethylformamide (DMF) and N-methyl-2-pyrrolidinone (NMP). However, the addition of a strong base, e.g. sodium hydroxide (NaOH) or sodium tert-butoxide increased the degree of coal dissolution in these organic solvents. Depending on the extraction conditions, carbon extraction efficiencies of up to 90% were obtained. Carbon precursor material was recovered from the solution as a gel by precipitation with water. Ash content was reduced from 10% in the coal to less than 1.6% in the coal extracts. Sodium sulfide (Na_2S) addition further reduced ash content and aided the recovery of carbon precursors that led to graphitizable cokes but the degree of extraction was significantly reduced.

10/00007 Elemental modes of occurrence in an Illinois #6 coal and fractions prepared by physical separation techniques at a coal preparation plant

Huggins, F. E. *et al. International Journal of Coal Geology*, 2009, 78, (1), 65–76.

In order to gain better insight into elemental partitioning between clean coal and tailings, modes of occurrence have been determined for a number of major and trace elements in an Illinois #6 coal and fractions prepared by physical separation methods at a commercial coal preparation plant. Elemental modes of occurrence were largely determined directly by XAFS or Mössbauer spectroscopic methods because the concentrations of major minerals and wt% ash were found to be highly correlated for this coal and derived fractions, rendering correlations between individual elements and minerals ambiguous for inferring elemental modes of occurrence. Of the major elements investigated, iron and potassium are shown to be entirely inorganic in occurrence. Most (90%) of the iron is present as pyrite, with minor fractions in the form of clays and sulfates. All potassium is present in illitic clays. Calcium in the original coal is 80–90% inorganic and is divided between calcite, gypsum, and illite, with the remainder of the calcium present as carboxyl-bound calcium. In the clean coal fraction, organically associated Ca exceeds 50% of the total calcium. This organically associated form of Ca explains the poorer separation of Ca relative to both K and ash. Among the trace elements, V and Cr are predominantly inorganically associated with illite, but minor amounts (5–15% Cr, 20–30% V) of these elements are also organically associated. Estimates of the V and Cr contents of illite are 420 ppm and 630 ppm, respectively, whereas these elements average 20 and 8 ppm in the macerals. Arsenic in the coal is almost entirely associated with pyrite, with an average As content of about 150 ppm, but some As (~10%) is present as arsenate due to minor oxidation of the pyrite. The mode of occurrence of Zn, although entirely inorganic, is more complex than normally noted for Illinois basin coals; about two-thirds is present in sphalerite, with lesser amounts associated with illite and a third form yet to be conclusively identified. The non-sulfide zinc forms are removed predominantly by the first stage of separation (rotary breaker), whereas the sphalerite is removed by the second stage (heavy media). Germanium is the only trace element determined to have a predominantly organic association.

10/00008 Experimental study of the effects of vegetable oil methyl ester on DI diesel engine performance characteristics and pollutant emissions

Lin, B.-F. *et al. Fuel*, 2009, 88, (9), 1779–1785.

Vegetable oil methyl ester (VOME) is produced through the transesterification of vegetable oil and can be used as biodiesel in diesel engines as a renewable, nontoxic, and potentially environmentally friendly fossil fuel alternative in light of growing concerns regarding global warming and increasing oil prices. This study used VOME fuels produced from eight commonly seen oil bases to conduct a series of engine tests to investigate the effects of VOME on the engine performance, exhaust emissions, and combustion characteristics. The experimental results showed that using VOME in an unmodified direct injection diesel engine yielded a higher brake specific fuel consumption (BSFC) due to the VOME fuel's lower calorific value. The high cetane number of VOME also imparted a better ignition quality and the high intrinsic oxygen content advanced the combustion process. The earlier start of combustion and the rapid combustion rate led to a drastic increase in the heat release rate (HRR) and the in-cylinder combustion pressure (ICCP) during the premixed combustion phase. A higher combustion rate resulted in higher peaks of HRR and ICCP as well as near the top dead centre position. Thus, it was found that a diesel engine fuelled with VOME could potentially produce the same engine power as one fueled with petroleum diesel, but with a reduction in the exhaust gas temperature (EGT), smoke and total hydrocarbon (THC) emissions, albeit with a slight increase in nitrogen oxides (NO_x) emissions. In addition, the VOME which possesses shorter carbon chains, more saturated bonds, and a higher oxygen content also yields a lower EGT as well as reduced smoke, NO_x, and THC emissions. However, this is obtained at the detriment of an increased BSFC.

10/00009 The remediation of MTE water by combined anaerobic digestion and chemical treatment

Artanto, Y. *et al. Fuel*, 2009, 88, (9), 1786–1792.

Mechanical thermal expression (MTE) is a developing process for the non-evaporative removal of water from low-rank coals prior to combustion. The water removed in this process contains both organic and inorganic components that would prevent its direct disposal to the environment. This study investigated the use of anaerobic digestion, in combination with ozonation and/or coagulation, to remediate MTE water. Under appropriate conditions the concentration of organic impurities, as determined by BOD, was reduced to be below guideline limits for release to surface waters. However, the electrical conductivity was increased to levels that would only permit its use for irrigation of salt tolerant plants with adequate drainage. Evidence of the effectiveness of remediation for organic carbon removal was also demonstrated by FTIR and pyrolysis-gas chromatography–mass spectrometry (Py-GC–MS). The latter revealed that the volatilizable organic components (aliphatic and aromatic hydrocarbons) were reduced by ~95% by anaerobic treatment.

Transport, storage

10/00010 Development of mixed conducting membranes for clean coal energy delivery

Leo, A. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (4), 357–367.

Mixed conducting membranes can be used for the separation of oxygen from air in both coal gasification and oxy-fuel power plants. In this review paper, the basic perovskite and non-perovskite structures, composition, properties and performance are addressed. Two typical perovskite materials, BSCF and LSCF, show promise in industrial applications as their oxygen fluxes are at least one order of magnitude higher than non-perovskite membranes. BSCF membranes are now delivering oxygen fluxes in excess of $5\,\mathrm{ml\,min^{-1}\,cm^{-2}}$. Latest developments in perovskite composition, effects of impurities in membrane performance and membrane geometry are discussed giving an insight into the potential utilization in clean energy delivery processes. Strategies for improving membranes performance using unit operations with different geometries and possible future technologies are also addressed.

10/00011 Effect of drilling fluids on coal permeability: impact on horizontal wellbore stability

Gentzis, T. *et al. International Journal of Coal Geology*, 2009, 78, (3), 177–191.

The study evaluates a series of mud systems and additives typically used in coalbed methane drilling in terms of formation of an instantaneous filter cake, ability of the coal reservoir to rid itself of the filter cake during production, and overall impact on coal permeability. A series of laboratory tests were conducted initially using artificially cleated gypstone rock (to simulate coal), followed by the use of large-diameter coal cores, which, unfortunately, did not allow for the tests to be done under *in situ* confining stress conditions. The three mud systems tested against coal (Xantham Gum, HEC and Na-CMC) did not have a negative impact on coal permeability, in contrast to previous laboratory data that showed large decreases. Two fluid loss control additives, which have been used successfully in drilling clastic and carbonate rocks, were also tested using a non-ionic polymer mud system. During simulated drilling, these additives (FLC 2000$^{\mathrm{TM}}$ and Q-Stop) were very effective in building a thin filter cake on the coal surface almost instantaneously, to the point that no solids were detected in the downstream fluid accumulator. During simulated production, a small pressure drop was sufficient to remove the filter cake. Coal permeability (to water) returned to its original (pre-test) value, which suggested that there was no permanent permeability damage caused by the two additives. When coal-derived fines were added to the drilling mud in another experiment using the same coal, the near wellbore coal permeability was reduced by 87.5%, indicating severe damage to the cleat system and in agreement with previously reported laboratory data. Following the very good performance of FLC 2000$^{\mathrm{TM}}$ and Q-Stop in the laboratory tests, these two additives were then used in field applications. Their presence in the drilling fluid resulted in the successful drilling of 953 m and 1400 m of total horizontal length in the deep Mannville coals in Alberta (at True Vertical Depth of 1400 m and 1150 m, respectively). No borehole instability problems were encountered during drilling of the two horizontal wellbores. The monitored mud losses were low in both cases, with the horizontal well #2 experiencing lower mud loss possibly as a result of the absence of large fractures encountered along the horizontal path. Horizontal well #1 remained stable, which allowed sufficient time to insert a production liner.

10/00012 From Scotia to Brookwood, fatal US underground coal mine explosions ignited in intake air courses

Dubaniewicz, T. H. *Journal of Loss Prevention in the Process Industries*, 2009, 22, (1), 52–58.

The National Institute for Occupational Safety and Health, Pittsburgh Research Laboratory, conducted a study of past mine explosions to identify the ignition locations and ignition sources responsible for the most severe explosion events resulting in death. Since the Scotia disaster of 1976, many fatalities from underground coal mine explosions have been linked to nonpermissible electrical equipment ignition sources located in intake air courses. With few exceptions, explosion protected equipment is generally not required in intake air courses of gassy underground coal mines in the USA. Cigarette lighters were another prevalent ignition source for fatal explosions ignited in intake air courses. Several mine rescue/recovery teams have encountered electrical ignition hazards. The study provides evidence that intake air courses of gassy underground coal mines fit the description of certain Hazardous (classified) locations described in the US National Electrical Code®. Class I Division 2 or Zone 2 explosion protection techniques may be used to design intake air equipment so that it does not present an ignition source under normal operation, before mine power is shut down in emergency situations. Nonpermissible circuits in intake air courses that are likely to remain energized during emergencies, e.g. battery powered equipment, should be protected by more stringent Class I Division 1, Zone 1, or Zone 0 techniques, to protect rescue/recovery personnel.

10/00013 Historical trends in American coal production and a possible future outlook

Höök, M. and Aleklett, K. *International Journal of Coal Geology*, 2009, 78, (3), 201–216.

The USA has a vast supply of coal, with almost 30% of world reserves and more than 1600 Gt (short) as remaining coal resources. The USA is also the world's second largest coal producer after China and annually produces more than twice as much coal as India, the third largest producer. The reserves are concentrated in a few states, giving them a major influence on future production. Historically many states have also shown a dramatic reduction in recoverable coal volumes and this has been closely investigated. Current recoverable estimates may also be too high, especially if further restrictions are imposed. The average calorific value of US coals has decreased from 29.2 MJ/kg in 1950 to 23.6 MJ/kg in 2007 as US production moved to subbituminous western coals. This has also been examined in more detail. This study also uses established analysis methods from oil and gas production forecasting, such as Hubbert linearization and logistic curves, to create some possible future outlooks for US coal production. In one case, the production stabilizes at 1400 Mt annually and remains there until the end of the century, provided that Montana dramatically increases coal output. The second case, which ignores mining restrictions, forecasts a maximum production of 2500 Mt annually by the end of the century.

Derived solid fuels

10/00014 Characterization of porous structure of coal char from a single devolatilized coal particle: Coal combustion in a fluidized bed

Sadhukhan, A. K. *et al. Fuel Processing Technology*, 2009, 90, (5), 692–700.

The combustion characteristics of coal char are highly dependent on initial pore structure of devolatilized char as well as on the structural evolution during the combustion of char. The development of pore structure also throws light on the mechanism of the combustion process. In the present work evolution of pore structure of partially burnt coal char of Indian origin has been investigated experimentally in a batch-fluidized bed and analysed. The BET surface area, micropore surface area and porosity of char at various levels of carbon burn-off have been determined. Experimental specific surface area has been found to agree well with theoretical prediction using random pore model. Modified random pore model is used to determine the active surface area. Char combustion mechanism based on shrinking unreacted core and shrinking reacted core models are delineated during the course of reaction at various bed temperatures. This is substantiated with the proportional representation of ash and carbon matrix in scanning electron microscope images. It is also concluded that in the present investigation the mean pore size is much smaller and hence the Knudsen diffusion predominates. Analysis based on similar experimental observations and models for pore structure evolution to investigate char combustion reaction regime has not been reported in literature.

10/00015 Experimental formation of massive hydrate deposits from accumulation of CH_4 gas bubbles within synthetic and natural sediments

Madden, M. E. *et al. Marine and Petroleum Geology*, 2009, 26, (3), 369–378.

In order for methane to be economically produced from the seafloor, prediction and detection of massive hydrate deposits will be necessary. In many cases, hydrate samples recovered from seafloor sediments appear as veins or nodules, suggesting that there are strong geologic controls on where hydrate is likely to accumulate. Experiments have been conducted examining massive hydrate accumulation from methane gas bubbles within natural and synthetic sediments in a large volume pressure vessel through temperature and pressure data, as well as visual observations. Observations of hydrate growth suggest that accumulation of gas bubbles within void spaces and at sediment interfaces likely results in the formation of massive hydrate deposits. Methane hydrate was first observed as a thin film forming at the gas/water interface of methane bubbles trapped within sediment void spaces. As bubbles accumulated, massive hydrate growth occurred. These experiments suggest that in systems containing free methane gas, bubble pathways and accumulation points likely control the location and habit of massive hydrate deposits.

10/00016 X-ray computed-tomography observations of water flow through anisotropic methane hydrate-bearing sand

Seol, Y. and Kneafsey, T. J. *Journal of Petroleum Science and Engineering*, 2009, 66, (3–4), 121–132.

This study used X-ray computed tomography (CT) to image and quantify the effect of a heterogeneous sand grain-size distribution on the formation and dissociation of methane hydrate, as well as the effect on water flow through the heterogeneous hydrate-bearing sand. A 28 cm long sand column was packed with several segments having vertical and horizontal layers with sands of different grain-size distributions. During the hydrate formation, water redistribution occurred. Observations of water flow through the hydrate-bearing sands showed that water was imbibed more readily into the fine sand, and that higher hydrate saturation increased water imbibition in the coarse sand due to increased capillary strength. Hydrate dissociation induced by depressurization resulted in different flow patterns with the different grain sizes and hydrate saturations, but the relationships between dissociation rates and the grain sizes could not be identified using the CT images. The formation, presence, and dissociation of hydrate in the pore space dramatically impact water saturation and flow in the system.

02 LIQUID FUELS

Sources, properties, recovery

10/00017 Analytical assessment of horizontal well efficiency with reference to improved oil recovery of the South-East Dragon oil field southern offshore of Vietnam

Quy, N. M. *et al. Journal of Petroleum Science and Engineering*, 2009, 66, (3–4), 75–82.

Nowadays, improved oil recovery (IOR) becomes much needed in field development planning, and is one of the main concerns for engineers in many reservoir management projects. Among IOR methods, horizontal wells have been widely applied in the world, and proved to be a promising technique. However, prudence is required in order to ensure maximum economic benefit in applying the technology. In this study, the applicability of horizontal well in the South-East Dragon field, which is a small fractured basement reservoir in the southern offshore of Vietnam, was assessed. An overview of the SE Dragon reservoir characteristics was provided. The potential performance of horizontal wells was analysed using analytical approaches, and the performance was compared with that predicted for vertical wells. Sensitivity study was conducted to investigate the effect of horizontal well length on well performance. The results of this study showed that, instead of a 350 m vertical well, drilling of a 400 m horizontal well at the same location could produce an additional 3,658,166 bbl of oil after 20 years. The efficiency increased proportionally with horizontal well length. The actual production rate can however be lower than predicted because of the assumptions used in the analysis.

10/00018 Application of integrated vitrinite reflectance and FAMM analyses for thermal maturity assessment of the northeastern Malay Basin, offshore Vietnam: implications for petroleum prospectivity evaluation

Petersen, H. I. *et al. Marine and Petroleum Geology*, 2009, 26, (3), 319–332.

Several exploration wells have intersected a Cenozoic coal-bearing, fluvial-deltaic mudstone and sandstone succession in the northeastern Vietnamese part of the Malay Basin, and have successfully tested seismically identified direct hydrocarbon indicators (DHIs). The oil and gas/condensate discovery well 46-CN-1x encountered an approximately 55 m thick section of lacustrine mudstones having considerable potential as an oil source. Vitrinite reflectance (VR) measurements from these alginite-bearing rocks introduce several problems in thermal maturity evaluation, including associated VR suppression and delineation of cavings and bitumens. Reliable thermal maturity gradients, however, may be established using a combination of conventional VR measurements and 'equivalent VR' (EqVR) values derived from the fluorescence alteration of multiple macerals (FAMM) technique. These measurements, performed on dispersed organic matter (DOM) in cuttings from 46-CN-1x, allow separation of low-reflecting bitumens and vitrinite in cavings from indigenous vitrinite and the FAMM results indicate VR suppression of 0.14% in an alginite-bearing mudstone with a high Hydrogen Index value. On the basis of available 'raw' VR data, a highly irregular maturity trend is determined, with the deepest sample (2675–2680 m) having a VR of approximately 0.4%R_o. The EqVR value, however, for the deepest sample is 0.70%. The maturity trend determined from the FAMM data (and VR data, omitting samples having suppressed VR) indicates that the top of the oil window (VR of 0.75%R_o) is located at about 2800 m depth. Modelling the geothermal gradient using the EASY%R_o algorithm yields approximately 40 °C/km for both of the two maturity profiles; this is in the low end of the range for the Malay Basin. Modelled temperature histories indicate onset of hydrocarbon generation for the uppermost Oligocene source rocks between 2 Ma and present-day, which post-dates trap formation. Seismic facies patterns suggest that lacustrine oil-prone units are in the oil window in the same graben complex a few km NW of the investigated well, and these rocks are likely to be the source of the hydrocarbons found in the well. A more widespread occurrence of hydrocarbons sourced from this kitchen is indicated by other discoveries and mapping of DHIs in the area.

10/00019 Appraisal of complex reservoirs with short-time tests

Raghavan, R. *et al. Journal of Petroleum Science and Engineering*, 2009, 66, (3–4), 165–170.

The utility of short-time tests to obtain the description of a reservoir with complex geology is evaluated. Using a porosity cube that is representative of the Brent reservoir in the North Sea, a series of independent tests is simulated and results are evaluated as a function of depth. The characteristics of the signatures are documented. An understanding of these signatures is particularly useful in that the overwhelming majority of the signatures is quite different from what is expected in REV-type models. Over 170 independent tests as a function of depth are evaluated, the permeability profile is computed and compared with the *in situ* profile and conclusions are derived. The conclusions that may be derived depend on the specifics of the model used to evaluate the pressure response. The fact that the estimation of permeability is a function of scale is recognized and attention is drawn to the fact that, if properly analysed, such tests must reflect scale dependency. Permeability estimates of short-time tests essentially yield values of permeability in the immediate vicinity of the perforation; thus, it is best to use data that represent local values to calibrate a model that reflects the underlying geology. Conventional interpretations will yield conservative estimates of well deliverability unless careful calibration is done with a model that carries the geological imprint.

10/00020 Black shale formation in the late Paleocene/early Eocene Arctic Ocean and paleoenvironmental conditions: new results from a detailed organic petrological study

Boucsein, B. and Stein, R. *Marine and Petroleum Geology*, 2009, 26, (3), 416–426.

The study of particulate organic matter (OM) in Arctic Ocean sediments from the late Cretaceous to the Eocene (IODP Expedition 302) has revealed detailed information about the aquatic/marine OM fluxes, biological sources, preservation and export of terrestrial material. Here, the authors present detailed data from maceral analysis, vitrinite reflectance measurements and organic geochemistry. During the Campanian/Paleocene, fluxes of land-derived OM are indicated by reworked and oxidized macerals (vitrinite, inertinite) and terrigenous liptinite (cutinite, sporinite). In the early Eocene, drastic environmental changes are indicated by peaks in aquatic OM (up to 40–45%, lamalginite, telalginite, liptodetrinite, dinoflagellate cysts) and amorphous OM (up to 50% bituminite). These events of increased aquatic OM flux, similar to conditions favoring black shale deposition, correlate with the global $\delta^{13}C$ events 'Paleocene/Eocene Thermal Maximum' (PETM) and 'Elmo event'. Freshwater discharge and proximity of the source area are documented by freshwater algae material (*Pediastrum, Botryococcus*) and immature land-plant material (corphuminite, textinite). The authors consider that erosion of coal-bearing sediments during transgression time lead to humic acids release as a source for bituminite deposited in the early Eocene black shales.

10/00021 Changes in gas composition during simulated maturation of sulfur rich type II-S source rock and related petroleum asphaltenes

Lehne, E. *et al. Organic Geochemistry*, 2009, 40, (5), 604–616.

Asphaltenes extracted from crude oils are proposed to possess structural features of the related source rock kerogen. For the present study micro-scale sealed vessel pyrolysis (MSSV) and combustion isotope ratio mass spectrometry (GC–C–IRMS) were used to compare gas generation from a whole rock (type II-S kerogen) from southern Italy with that from related sulfur rich asphaltenes isolated from a low maturity heavy crude oil. The purpose of was to determine whether experimental pyrolysis of oil asphaltenes can be used to predict the timing and the chemical and isotopic composition of hydrocarbon gases generated from genetically related kerogen in the source rock during burial maturation. The results show that parameters such as gas-to-oil ratio (GOR) and oil and gas formation timing are very similar for these two sample types, whereas gas composition, product aromaticity and sulfur content are remarkably different. Slight differences in GOR are mainly due to differences in gas formation characteristics at very high levels of thermal alteration. Secondary gas formation from the whole rock covers a much broader temperature range under geological conditions than that from the asphaltene products. However, it is remarkable that both the onset and the maximum temperature are nearly identical under geological conditions. The observed differences in gas generation characteristics are supported by discrepancies in the carbon isotopic characteristics of the gas range compounds and indicate different precursors and/or mechanisms for gas generated from whole rock and asphaltenes.

10/00022 Composition, peat-forming vegetation and kerogen paraffinicity of Cenozoic coals: relationship to variations in the petroleum generation potential (Hydrogen Index)

Petersen, H. I. *et al. International Journal of Coal Geology*, 2009, 78, (2), 119–134.

Coals with similar thermal maturity and from the same deposit normally show a considerable range in petroleum generation potential as measured by the Hydrogen Index (HI). Some Cenozoic coals and coaly sediments have the potential to generate oil, which is related to the coal's paraffinicity. Coal paraffinicity is not readily reflected in the bulk HI. In this paper, the relationships between measured HI and coal composition, coal kerogen paraffinicity and floral input have been investigated in detail for three sets of coals from Colombia/Venezuela, Indonesia, and Vietnam. The samples in each coal set are largely of iso-rank. The petroleum generation potential was determined by Rock–Eval pyrolysis. Reflected light microscopy was used to analyse the organic matter (maceral) composition and the thermal maturity was determined by vitrinite reflectance (VR) measurements. The botanical affinity of pollen and spores was analysed by palynology. Coal kerogen paraffinicity was determined by ruthenium tetroxide-catalysed oxidation (RTCO) followed by chain length analysis and quantification (mg/g TOC) of the liberated aliphatic chains. The coals are dominated by huminite, in particular detrohuminite. Only the Vietnamese coals are rich in microscopically visible liptinite. The pollen and spores suggest that the coals were derived principally from complex angiosperm mire vegetations, with subordinate proportions of ferns that generally grew in a subtropical to tropical climate. Measured HI values vary considerably, but for the majority of the coals the values lie between approximately 200 mg HC/g TOC and 300 mg HC/g TOC. Aliphatics yielding monocarboxylic acids dominate in the coal kerogen, whereas aliphatics yielding dicarboxylic acids are secondary. However, the dicarboxylic acids show that cross-linking long-chain aliphatics are present in the kerogen structure. All studied coals are paraffinic with C_{19-35} aliphatic chains in the kerogen, and the aliphatics in the range C_{25-35} show that the coals may have the potential to generate waxy crude oil. The Indonesian coals are richest in long-chain aliphatics and are thus potentially most oil-prone. The present three sample sets variations in HI are positively correlated to different combinations of the C_{10+} aliphatic chains in the kerogen and the amount of detrohuminite + liptodetrinite and liptinite. Furthermore, part of the HI can be attributed to hydrogen in compounds with less than 10 carbon atoms, which is the lowest alkyl detected by RTCO analysis, thus representing a potential for generation of gas and light liquid hydrocarbons. The measured HI is therefore not always a good indicator for humic coal's potential to source waxy oil. Vegetational influence (palynology) on the variation of HI cannot be shown within the investigated span of variance and for the present coals. However, it is likely that some of the range in measured HI values is caused by floral variations not revealed by the palynological analysis and to variations in the preservation of the organic matter.

10/00023 Effect of S-compounds on Pd over $LaMnO_3 \cdot 2ZrO_2$ and $CeO_2 \cdot 2ZrO_2$ catalysts for CH_4 combustion

Specchia, S. *et al. Catalysis Today*, 2009, 143, (1–2), 86–93.

The ageing effect induced by S-compounds (added as odorants in the natural gas network for safety purposes) over 2% Pd/$LaMnO_3 \cdot 2ZrO_2$ and 2% Pd/$CeO_2 \cdot 2ZrO_2$ catalysts for methane combustion is studied. The catalysts were prepared by solution combustion synthesis (SCS), starting from metal nitrates/glycine mixtures. Basic characterization

(XRD, BET, FESEM/EDS, TPD/TPR analysis), FT-IR studies and catalytic activity tests were performed on powder catalysts in fresh status and after accelerated ageing carried out up to 3 weeks (hydrothermal treatment at 800 °C under a flow of domestic boiler exhaust gases typical composition (9% CO_2, 18% H_2O, 2% O_2 in N_2), also including 200 ppmv of SO_2 to emphasize any poisoning effect). After ageing, 2% Pd/$CeO_2{\cdot}2ZrO_2$ increased its methane combustion half-conversion temperature (T_{50}), regarded as an index of catalytic activity, from 382 °C – recorded for fresh sample – to 490 °C. An unexpected improvement in the overall performance was found instead for 2% Pd/$LaMnO_3{\cdot}2ZrO_2$: T_{50}, in fact, got lowered from 570 °C (fresh sample) to 465 °C (after 3 weeks ageing). S-hydro-thermal treatment induced bulk and surface sulfates formation on all aged samples, with a concentration increasing with the exposure time. The prevailing ageing mechanisms seemed to be the oxidation of Pd metallic clusters, detected over the Ce–Zr system, and the formation of surface-bulk sulfates, the latter destroying the initial crystallographic structure, particularly evident for the La–Mn system. The increased activity of the 2% Pd/$LaMnO_3{\cdot}2ZrO_2$ sample could be explained with the formation of MnO_x, detected via XRD and IR, which is active towards methane combustion.

10/00024 Investigating the performance of hot water injection in geostatistically generated permeable media

Alajmi, A. F. *et al. Journal of Petroleum Science and Engineering*, 2009, 66, (3–4), 205–869.

The study investigates the performance of hot water flooding compared to conventional water flooding in recovering heavy oil from heterogeneous reservoirs through fine-mesh numerical simulations. A total of 16 permeability maps were generated geostatistically to cover a wide range of reservoir heterogeneity. Two measures of heterogeneity were used to characterize the permeability maps: the Dykstra–Parsons coefficient and the spatial correlation length. Extensive three-dimensional, fine-mesh simulation runs were performed to study the functional relationships between several design parameters and the oil recovery obtained during hot water flooding. These results were then compared to those obtained by conventional water flooding. Parameters which were investigated include: (1) degree of reservoir heterogeneity (2) injected fluid temperature (3) well configurations, and (4) viscosity ratio. Results showed that these parameters play important roles in the displacement behaviour of heavy oil, with reservoir heterogeneity having more significant effects. It is proven that hot water flooding can be more effective than conventional one by considering the critical values of the above studied parameters. The paper also shows the conditions that can be detrimental to hot water flooding.

10/00025 Isothermal vapor–liquid equilibrium at 333.15 K, excess molar volumes and refractive indices at 298.15 K for mixtures of *tert*-amyl methyl ether + ethanol + 2,2,4-trimethylpentane

Hwang, I.-C. *et al. Fluid Phase Equilibria*, 2009, 281, (1), 5–11.

Isothermal vapour–liquid equilibrium data at 333.15 K are measured for the binary system *tert*-amyl methyl ether + ethanol and *tert*-amyl methyl ether + 2,2,4-trimethylpentane and for ternary system *tert*-amyl methyl ether + ethanol + 2,2,4-trimethylpentane by using headspace gas chromatography. The experimental vapour–liquid equilibrium data were correlated with G^E models (Margules, van Laar, Wilson, NRTL, UNIQUAC) equations. The excess volume and deviations in molar refractivity data are also reported for the same binary and ternary systems at 298.15 K. These data were correlated with the Redlich–Kister equation for the binary systems and the Cibulka equation for the ternary system, respectively. The experimental ternary excess volume and deviations in molar refractivity data, were also compared with the estimated values from the binary contribution models of Tsao–Smith, Kohler, Rastogi and Radojkovic.

10/00026 Modelling an atypical petroleum system: a case study of hydrocarbon generation, migration and accumulation related to igneous intrusions in the Neuquen Basin, Argentina

Monreal, F. R. *et al. Marine and Petroleum Geology*, 2009, 26, (4), 590–605.

Immature source rock sections in the Neuquen Basin in Argentina intruded by up to 600 m thick Tertiary laccoliths show full spectrum maturity aureoles over hundreds of metres from the contacts. Commercial oil accumulations (20–33°API) and oil shows are located along the entire column, both in sandstone/carbonate and fractured igneous reservoirs. A two-dimensional petroleum system model achieved satisfactory results when accounting for thermal maturation, oil and gas generation, composition, migration, and known accumulations. This atypical petroleum system is characterized by thermal anomalies lasting thousands of years that are the result of the progressive cooling of the igneous intrusions. Host source rocks were exposed to a wide range of temperatures that varied in time and space generating different maturity products. High generation pressures, source rock fracturation, and convective water flows facilitated migration and mixing of hydrocarbons and the charge of the igneous bodies as they were fractured during thermal contraction. Oil and source rock analyses were done in order to calibrate and support modelling results. Geochemical correlations suggest an *in situ* generation related to the igneous intrusions. In particular, diamondoids' measurements show mixing processes of high-mature (cracked) with low-mature hydrocarbons. Oils generated and cracked close to the laccoliths and oils generated from more distant source rock sections, less affected by the thermal anomalies, were probably mixed as they migrated towards the igneous bodies and shallower reservoirs. The integration of a wide set of geochemical analyses and recent modelling techniques based upon time and temperature calculation performance enhancements, led to novel insights on this atypical petroleum system.

10/00027 Multistring analysis of wellhead movement

Aasen, J. A. and Aadnoy, B. S. *Journal of Petroleum Science and Engineering*, 2009, 66, (3–4), 111–116.

This paper presents simple models to describe casing loading and wellhead movement during both the installation (mechanical) phase as well as the production (thermal) phase. Input parameters include hook load during installation and temperature change during production. The theory is simple and the formulations are suitable for hand-calculations and spreadsheet. The presented models are applicable to both conventional and HP/HT (high-pressure/high-temperature) wells. The term multistring analysis refers to the involved casing strings which are connected at the wellhead and therefore, the applied mechanical or thermal disturbances will cause wellhead movement that depends upon the interaction of the different tubulars. A field case is presented and analysed using presented theory. This is an offshore well where the wellhead suddenly dropped several feet due to a collapsed surface casing. The incident took place during wellhead cooling following a routine shutdown. The expected wellhead contraction due to cooling did not occur. After an extended period with no wellhead movement, the wellhead suddenly released. A corroded segment of the surface casing collapsed and the wellhead dropped.

10/00028 Practical kinetic modelling of petroleum generation and expulsion

Stainforth, J. G. *Marine and Petroleum Geology*, 2009, 26, (4), 552–572.

Models for petroleum generation used by the industry are often limited by (a) sub-optimal laboratory pyrolysis methods for studying hydrocarbon generation, (b) over-simple models of petroleum generation, (c) inappropriate mathematical methods to derive kinetic parameters by fitting laboratory data, (d) primitive models of primary migration/expulsion and its coupling with petroleum generation, as well as (e) insufficient use of subsurface data to constrain the models. Problems (a), (b) and (c) lead to forced compensation effects between the activation energies and frequency factors of reaction kinetics that are wholly artificial, and which yield poor extrapolations to geological conditions. Simple switch or adsorption models of expulsion are insufficient to describe the residence time of species in source rocks. Yet, the residence time controls the thermal stresses to which the species are subjected for cracking to lighter species. The ShellGenex model for petroleum generation and expulsion has been developed since 1988. In this multi-species model, the rate-limiting step of primary migration is treated as the slow diffusion of the petroleum through the kerogen itself. Other key aspects of the model are: the reaction and transport behaviour of the heavy compounds; the role of free radicals in the cracking kinetics of hydrocarbon species in the model; and the evolving free volume of the kerogen. The last of these has a particularly strong effect on the primary migration of the generated petroleum molecules. Some implications of this model are that (a) compositions of expelled petroleum vary more strongly than the standard parallel-reaction model suggests, and (b) expulsion is not immediately extinguished by waning temperatures and pressures, but continues with decreasing GOR of the expelled petroleum and increasing density of the expelled oil.

10/00029 Spontaneous imbibition of seawater into preferentially oil-wet chalk cores – experiments and simulations

Yu, L. *et al. Journal of Petroleum Science and Engineering*, 2009, 66, (3–4), 171–179.

Spontaneous imbibition is an important improved oil recovery (IOR) process, especially for fractured carbonate reservoirs with low permeability matrix blocks. If the chalk is oil-wet, the process will not take place. Previous studies have shown that seawater may increase the water-wetness. The sulfate ions in seawater may alter the wetting conditions of the chalk surface, especially at high temperatures. One-dimensional imbibition tests of water into vertically placed, preferentially oil-wet chalk cores were performed, with non-sulfate formation water as a reference. The cores were sealed and only open to flow at one or both end faces. For core plugs with both ends open, a delay period was observed if the core initially was 100% oil saturated, and the difference in oil recovery from top and bottom was about 2–4% of OOIP. For core plugs with initial water saturation, the difference was increased to 14% of OOIP with higher oil production from the top. For cores with only the upper end face open to flow, only countercurrent imbibition takes place. Higher oil recovery was observed with seawater than with formation water as imbibing brine. Cleaned core plugs can be more easily rendered partially oil-wet. A numerical model was developed to describe the seawater imbibition process, including the effect of wettability alteration, and used to simulate the experiments. The model includes molecular diffusion and adsorption of salts (sulfate), and gravitational and capillary forces. The salts in the seawater diffuse into the formation water initially present in the core, absorb onto the rock surface and induce wettability alteration. Two measured capillary pressure curves are used in the simulation. The curve with seawater is taken as the water-wet extreme, and the curve with non-sulfate formation water is taken as the oil-wet extreme. The capillary pressure curve is dynamically shifted from oil-wet to water-wet conditions proportionally to the absorb amount of salt. The simulation results match the experimental data well. The inclusion of the dynamic shift of the wettability condition controlled by molecular diffusion results in delayed oil recovery, in line with the experimental results. The model can easily be extended to include different types of ion concentration, e.g. of magnesium and calcium, to include more of the chemical reactions taking place.

10/00030 The influence of viscosity on stability of foamy oil in the process of heavy oil solution gas drive

Wang, J. *et al. Journal of Petroleum Science and Engineering*, 2009, 66, (1–2), 69–74.

Primary production from some heavy-oil reservoirs in the process of solution gas drive exhibits high primary recovery. This is because the formation and flow of foamy oil which indicated that gas was dispersed in the heavy oil and flow with oil phase when formation pressure was lower than bubble pressure. The stability of foamy oil was influenced by many issues including oil viscosity, the contents of dissolved gas, temperature and the pressure depletion rate. The authors mainly researched the influence of oil viscosity on stability of foamy oil in the process of heavy oil solution gas drive. Through sand-pack experiment, foam quality and half-life period of foamy oil were researched for different oil viscosity under atmosphere pressure and temperature of 25 °C, neglecting pressure depletion rate. Results indicated that as oil viscosity increased, the stability of foamy oil became better. Large solution viscosity plays an important role in retarding the transport of gas from solution to the growing bubble in the foamy oil because bubble volume increases much more slowly in viscous oils, coalescence is slowed dramatically. The curve between half-life period and oil viscosity had an inflection point and its corresponding oil viscosity can be used as proper viscosity suitable for heavy oil solution gas drive and sand-carrying cold production.

10/00031 The oxidation of a gasoline surrogate in the negative temperature coefficient region

Lenhert, D. B. *et al. Combustion and Flame*, 2009, 156, (3), 549–564.

This experimental study investigated the preignition reactivity behaviour of a gasoline surrogate in a pressurized flow reactor over the low and intermediate temperature regime (600–800 K) at elevated pressure (8 atm). The surrogate mixture, a volumetric blend of 4.6% 1-pentene, 31.8% toluene, 14.0% *n*-heptane, and 49.6% 2,2,4-trimethyl-pentane (iso-octane), was shown to reproduce the low and intermediate temperature reactivity of full boiling range fuels in a previous study. The surrogate components were examined to identify the major intermediate species in order to improve existing kinetic models, where appropriate, and to provide a basis for examining constituent interactions in the surrogate mixture. *n*-Heptane and 1-pentene started reacting at 630 K and 640 K, respectively, and both fuels exhibited a strong negative temperature coefficient (NTC) behaviour starting at 700 and 710 K, respectively. Iso-octane showed a small level of reactivity at 630 K and a weak NTC behaviour starting at 665 K. Neat toluene was unreactive at these temperatures. The surrogate started reacting at 630 K and exhibited a strong NTC behaviour starting at 693 K. The extent of fuel consumption varied for each of the surrogate constituents and was related to their general autoignition behaviour. Most of the intermediates identified during the surrogate oxidation were species observed during the oxidation of the neat constituents; however, the surrogate mixture did exhibit a significant increase in intermediates associated with iso-octane oxidation, but not from *n*-heptane. While neat toluene was unreactive at these temperatures, in the mixture it reacted with the radical pool generated by the other surrogate components, forming benzaldehyde, benzene, phenol, and ethyl-benzene. The observed *n*-heptane, iso-octane, and surrogate oxidation behaviour was compared to predictions using existing kinetic models. The *n*-heptane model reasonably predicted the disappearance of the fuel, but overpredicted the formation of several of the smaller intermediates. The iso-octane model significantly overpredicted the reaction of the fuel and formation of the intermediates. The 1-pentene model reasonably predicted the fuel consumption, but underestimated the importance of radical addition to the double bond.

Transport, refining, quality, storage

10/00032 Assessment of local thin areas in a marine pipeline by using the FITNET FFS corrosion module

Cicero, S. *et al. International Journal of Pressure Vessels and Piping*, 2009, 86, (5), 329–334.

This paper analyses the structural integrity of the marine stretch of a pipeline, which is placed over a natural bay. The pipeline is part of a 30-year-old installation used for the provision of petrochemical products to a nearby chemical plant. Although there have been no relevant leaks in the past, both the visual inspections performed (revealing numerous local thin areas) and the fact that it is located in a highly sensitive place with high ecological and tourist value recommend the assessment of the pipeline in order to ensure that it is working in safe conditions and that there are no risks for the environment or the people living in the surrounding area. The assessment has been performed using the newly developed FITNET FFS procedure, whose local thin areas assessment methodology is also explained and compared to the analyses proposed by other well-known procedures.

10/00033 Chemical desulfurization of petroleum fractions for ultra-low sulfur fuels

Ali, M. F. *et al. Fuel Processing Technology*, 2009, 90, (4), 536–544.

An improved desulfurization process for removing sulfur from hydro-treated diesel oil based on the oxidation of thiophenic type sulfur-containing compounds with H_2O_2 and acetic acid (AcOH) using H_2SO_4 as a catalyst has been studied. The experimental results show that the sulfone content in the oxidation product increased rapidly with an increase in acetic acid and sulfuric acid ratios from 1:0 to 2:1 mole ratios. The maximum DBT conversion (wt%) was at 2:1 mole ratio of acetic acid/sulfuric acid. This oxidation process is found to be capable of removing up to 90% of the sulfur compounds in hydro-treated real fuels and can provide an alternative way to meet the future sulfur environmental requirements. Fifty-eight sulfur-containing compounds were identified in the hydro-treated diesel sample. These include mainly refractory sulfur compounds (thiophenes and multi-ring aromatic sulfur compounds, such as dibenzothiophene (DBT)). Sulfur species in typically hydro-treated diesel and ring number distribution in 254–385 °C cut are also reported.

10/00034 Design and off-design analyses of a pre-combustion CO_2 capture process in a natural gas combined cycle power plant

Nord, L. O. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (4), 385–392.

In this study, a cycle designed for capturing the greenhouse gas CO_2 in a natural gas combined cycle power plant has been analysed. The process is a pre-combustion CO_2 capture cycle utilizing reforming of natural gas and removal of the carbon in the fuel prior to combustion in the gas turbine. The power cycle consists of a H_2-fired gas turbine and a triple pressure steam cycle. Nitrogen is used as fuel diluent and steam is injected into the flame for additional NO_x control. The heat recovery steam generator includes pre-heating for the various process streams. The pre-combustion cycle consists of an air-blown auto-thermal reformer, water–gas shift reactors, an amine absorption system to separate out the CO_2, as well as a CO_2 compression block. Included in the thermodynamic analysis are design calculations, as well as steady-state off-design calculations. Even though the aim is to operate a plant, as the one in this study, at full load there is also a need to be able to operate at part load, meaning off-design analysis is important. A reference case which excludes the pre-combustion cycle and only consists of the power cycle without CO_2 capture was analysed at both design and off-design conditions for comparison. A high degree of process integration is present in the cycle studied. This can be advantageous from an efficiency stand-point but the complexity of the plant increases. The part load calculations is one way of investigating how flexible the plant is to off-design conditions. In the analysis performed, part load behaviour is rather good with efficiency reductions from base load operation comparable to the reference combined cycle plant.

10/00035 Hydroprocesssing of light gas oil – rape oil mixtures

Walendziewski, J. *et al. Fuel Processing Technology*, 2009, 90, (5), 686–691.

Two series of experiments of hydroprocessing of light gas oil–rape oil mixtures were carried out. The reactor feed was composed of raw material: first series 10 wt% rape oil and 90 wt% of diesel oil; second series 20 wt% rape oil and 80 wt% of diesel oil. Hydroprocessing of both mixtures was performed with the same parameter sets, temperature (320, 350 and 380 °C), hydrogen pressure 3 and 5 MPa, $LHSV = 2\,h^{-1}$ and hydrogen feed ratio of $500\,Nm^3/m^3$. It was stated that within limited range it is possible to control vegetable oil hydrogenolysis in the presence of light gas oil fraction (diesel oil boiling range) through the proper selection of the process parameters. Hydrogenolysis of ester bonds and hydrogenation of olefinic bonds in vegetable oils are the main reactions in the process. Basic physicochemical properties of the obtained hydroprocessed products are presented.

10/00036 Improving the gasoline quality of liquid products from the Fisher–Tropsch process

Madikizela-Mnqanqeni, N. N. *Catalysis Today*, 2009, 143, (1–2), 126–131.

The un-fractionated, un-hydrotreated liquid fractions from the high temperature Fisher–Tropsch (HTFT) process was aromatized over HZSM-5 catalysts at different reaction temperatures and pressures to determine the impact. The flame ionization detector–gas chromatography results indicated that there were high amounts of aromatic and BTX (benzene, toluene, and xylenes) compounds contained in the gasoline fraction at a reaction temperature between 400 and 425 °C. Over a period of 6 days of TOL, the estimated research octane numbers of different streams ranged between 102 and 93 and motor octane numbers between 92 and 80. The research octane numbers and motor octane numbers values of the streams resulting from the aromatization reaction indicated an improvement in octane and hence improved the blend ability or the component.

10/00037 Interactions between oil shale and its semi-coke during co-combustion

Wang, Q. *et al. Fuel*, 2009, 88, (8), 1520–1529.

Thermogravimetric analysis was used in this study to investigate the interactions between oil shale and its semi-coke during co-combustion process. During the test, the blends of semi-coke and oil shale were prepared at different blending ratios of 1:0, 4:1, 3:1, 2:1, 1:1, and 0:1. The results indicated some interactions were detected between oil shale and semi-coke during the tests. The rapid combustion of organic matter in oil shale, which led to the fuel particle temperature's rapid increase and made semi-coke ignite in advance, improved the co-combustion characteristics in terms of ignition temperature (T_i), the temperature reaching the maximum mass loss rate (T_{max}), the maximum mass loss rate (R_{max}), the combustibility index (C) and the specific reactivity of the co-combustion. With the increase in semi-coke mass fraction in the blends, the specific reactivity of the samples was found to decrease gradually due to lower volatile content and high carbon condensation structure in semi-coke. As the temperature increased, the specific reactivity of the samples first gradually increased, then decreased attributed to the oxidation of selectivity. The poor diffusion caused mainly by the ash shells made the decomposition of minerals more complicated. It was also analysed that the 'particle groups' phenomenon that the dispersed particles are agglomerated by some forces in semi-coke ash went against the decomposition of minerals. Activation energies E from distributed activation energy (DAEM) slowly decreased at the initial stage, then increased sharply over a narrow conversion region, which indicted a difficult burnout stage. Meantime, a power law model was employed to investigate quantitatively the interactions. The experimental reaction orders could be predicted accurately from the calculated values. At the third stage, the kinetic parameters E_3 and A_3 were almost as much as the calculated values. At the low temperature region (470–540 °C), there was little difference between kinetic parameters E and A from the experiment data and the calculated data.

10/00038 Microemulsion flooding for enhanced oil recovery

Santanna, V. C. *et al. Journal of Petroleum Science and Engineering*, 2009, 66, (3–4), 117–120.

Petroleum recovery methods basically consist of fluid injection aiming to displace the oil out of the rock pores. Among the methods used in enhanced oil recovery, chemical methods, which may involve microemulsion flooding, are cited. In this work, injection assays have been carried out with two types of microemulsion: one was prepared with a commercial surfactant (MCS) and another contained a surfactant synthesized in laboratory (MLS). The experiments basically consisted of the injection of fluids into cylindrical plug samples from the Assu Formation (RN, Brazil). During the microemulsion flooding, samples were collected as a function of time and the mass of oil recovered by the microemulsion was determined. From the results obtained, one could conclude that the use of microemulsion prepared with the commercial MCS allowed for recovery indices as high as 87.5%, whilst the use of the MLS microemulsion permitted recovery indices as high as 78.7%. This was mainly due to the difference in viscosity between the two microemulsions used.

10/00039 Neuro-based formulation to predict fouling threshold in crude preheaters

Aminian, J. and Shahhosseini, S. *International Communications in Heat and Mass Transfer*, 2009, 36, (5), 525–531.

For preheat exchangers of a crude distillation unit (CDU), operating in conditions such that fouling minimized is crucial. A number of semi-empirical models called 'threshold fouling models' were developed by various researchers to predict crude oil fouling behaviour in crude preheaters of CDUs. In this study, an artificial neural network (ANN) model has been employed to develop a set of mathematical formulations to identify regions where there is less/no fouling. The comparisons between results of the developed neuro-based formulation and three threshold fouling models showed the use of neuro-based model resulted in significant improvements in terms of predicting crude oil fouling behaviour of various laboratory and plant data. The approach of developing neuro-based models to predict fouling behaviour can be readily applied in CDUs to identify more accurate fouling/no-fouling operating zones leading to an enhancement in the operation of crude preheaters.

10/00040 Optimal rectification column, reboiler vessel, connection pipe selection and optimal control of batch distillation considering hydraulic limitations

Simon, L. L. *et al. Chemical Engineering and Processing: Process Intensification*, 2009, 48, (4), 938–949.

In this paper the optimal selection of the reboiler vessels, rectification columns and connection pipes with regard to reboiler swelling, and tray and pipe flooding is investigated. Since the reboilers are constrained by liquid swelling, while pipes and columns are constrained by flooding it is important to pair the equipment so that the vapour rate limitations are as close as possible, thus ensuring maximal equipment capacity usage. Calculations at 1 and 0.25 bar pressure are performed for the standardized 1.6, 2.5, 4 and $6.3\,m^3$ reboiler vessels (Rührbehälter Basler Norm, N 253, 1977) and sieve tray rectification columns with nominal diameters ranging from 0.2 up to 0.6 m. The dynamic operation of the batch distillation process having the vapour load and reflux ratio as input profiles is evaluated by formulating and solving an optimal control problem constrained by the hydraulic limitations. The open-loop optimization problem is solved using a dedicated Matlab tool – OptCon – which implements the multiple shooting strategy and the large-scale non-linear programming problem is handled by the HQP engine.

10/00041 Retrofit of sour water networks in oil refineries: a case study

Sujo-Nava, D. *et al. Chemical Engineering and Processing: Process Intensification*, 2009, 48, (4), 892–901.

A case study is presented of the retrofit of a sour water network in a petroleum refinery that generates $581{,}000\,m^3$/yr of sour water. Flowrates and contaminant levels of ammonia and hydrogen sulfide were traced for all major water streams in the sour water network. By grouping some process units, a reuse scheme was found that only generates $280{,}000\,m^3$/yr of sour water, saving 83% of freshwater and 52% in energy and CO_2 emissions associated with pumping and the heat requirement to scrub out the sour components. Additionally, it was found that the remaining water, after treatment in the sour water stripper, could be reused elsewhere in the plant, if cyanide ions were eliminated. This case study has provided the foundation for further plant studies to validate the water profile of the proposed scheme.

10/00042 The analysis and prediction of scale accumulation for water-injection pipelines in the Daqing Oilfield

Liu, X. *et al. Journal of Petroleum Science and Engineering*, 2009, 66, (3–4), 161–164.

In the process of development in the Daqing Oilfield, scale has been produced in water-injection pipelines. The process, mechanism and influencing factors of scaling are discussed, and the main type of the scale in water-injection pipelines of the forth plant of the Daqing Oilfield is analysed. The saturation index method and the thermodynamics solubility method were adopted to predict the tendency of scaling. Moreover, the precautionary and control measures of scaling in oilfield pipeline.

10/00043 Transition metal phosphide hydroprocessing catalysts: a review

Oyama, S. T. *et al. Catalysis Today*, 2009, 143, (1–2), 94–107.

The diminishing quality of oil feedstocks coupled with increasingly more stringent environmental regulations limiting the content of sulfur in transportation fuels have given rise to a need for improved hydroprocessing technology. This review begins with a summary of the major improvements in hydrodesulfurization (HDS) and hydrodenitrogenation (HDN) catalysts and processes that have been reported in recent years. It then describes a new class of hydroprocessing catalysts, the transition metal phosphides, which have emerged as a promising group of high-activity, stable catalysts. The phosphides have physical properties resembling ceramics, so are strong and hard, yet retain electronic and magnetic properties similar to metals. Their crystal structures are based on trigonal prisms, yet they do not form layered structures like the sulfides. They display excellent performance in HDS and HDN, with the most active phosphide, Ni_2P, having activity surpassing that of promoted sulfides on the basis of sites titrated by chemisorption (CO for the phosphides, O_2 for the sulfides). In the HDS of difficult heteroaromatics like 4,6-dimethyldibenzothiophene Ni_2P operates by the hydrogenation pathway, while in the HDN of substituted nitrogen compounds like 2-methylpiperidine it carries out nucleophilic substitution. The active sites for hydrogenation in Ni_2P have a square pyramidal geometry, while those for direct hydrodesulfurization have a tetrahedral geometry. Overall, Ni_2P is a promising catalyst for deep HDS in the presence of nitrogen and aromatic compounds.

Economics, business, marketing, policy

10/00044 3D hydrocarbon migration by percolation technique in an alternate sand–shale environment described by a seismic facies classified volume

Corradi, A. *et al. Marine and Petroleum Geology*, 2009, 26, (4), 495–503.

Modelling hydrocarbon migration in complex depositional environments is a difficult task. This paper illustrates a workflow that has been developed in order to make use of information at seismic resolution for migration modelling purposes. After a regional identification of the main seismic sequence boundaries and systems tracts, the first step of the workflow consists in a semi-automatic classification of the sand and shale prone seismic facies that are interpretable in the seismic volume. Software based on supervised neural network techniques and textural seismic attributes supports volumetric classification. Each class represents a different facies with specific petrophysical properties, assigned according to concurrent sedimentological studies; the result is a 3D lithofacies model. Petroleum system modelling is performed on a 3D regional model up to the calculation of hydrocarbon quantities expelled from the source rock. Then migration modelling is performed on the smaller area covered by the 3D lithofacies model. Invasion percolation approach has been chosen because it allows migration modelling to be performed at a scale that is small enough to maintain a sufficient detail of the channels' shape and of their connections. A probabilistic approach allows charge risk in new prospects to be estimated and modelling consistency to be checked. This workflow has been applied in a deep water setting in West Africa, characterized by an interconnected channel system, where a number of prospects had to be evaluated. A well was drilled in the area prior to this study, resulting dry in spite of being located in a position where the source rock is present and is deemed to have expelled interesting amounts of hydrocarbons. This study shows that hydrocarbons expelled from the source appear to be deviated laterally by the presence of a local seal and therefore do not reach the channel system in the well location.

10/00045 Causality relationship between the price of oil and economic growth in Japan

Hanabusa, K. *Energy Policy*, 2009, 37, (5), 1953–1957.

This paper investigates the relationship between the price of oil and economic growth in Japan during the period from 2000 to 2008 using an exponential generalized autoregressive conditional heteroskedasticity (EGARCH) model. A residual cross-correlation function approach, developed in an earlier study was also employed. The empirical results reveal that the economic growth rate Granger-causes the change of oil price in mean and variance and the change of oil price Granger-causes the economic growth rate in mean and variance. Previous studies have analysed the response of economic activity to oil price shocks. However, the causality relations are analysed for both means and variances are analysed, and identify the direction of information flow and the timing of causation.

10/00046 Environmental problems in the Estonian oil shale industry

Raukas, A. and Punning, J.-M. *Energy Environmental Science*, 2009, 2, (7), 723–728.

In Estonia technologies for oil shale mining and consuming have been continuously developed for more than 80 years. By March 2006 one billion tonnes of oil shale had been produced in Estonia. Since the 1960s, Estonia has been the largest oil shale producer and consumer in the world. In the 1980s about two-thirds of the world's oil shale output came from Estonia. Serious problems in the mining complex are connected with large losses of oil shale at mining and enrichment (more than 30%) and voluminous dewatering ($25\,m^3$ per tonne of oil shale). After mining and beneficiation, much limestone remains unused and is deposited in waste dumps. Oil shale waste and waste heaps may be considered a rather innocent production residue; however, from time to time they are subject to self-ignition. Following combustion of enriched oil shale, ash remains which also has to be deposited. The most toxic waste (semicoke) comes from the oil-shale chemical industry. Power stations using oil shale emit large amounts of carbon dioxide and other gases; the groundwater regime, and often also the water quality, are altered in mined-out areas. Environmental effects and the resulting immediate hazards were greatest in the 1980s, now the situation is improving.

10/00047 Latin America battles geology and politics to prevent decline in oil production; part 1

Anon., *Oil and Energy Trends*, 2009, 34, (6), 3–6.

The importance of Latin America as an important global oil supplier, particularly to the USA and more recently China, is firmly established and demand looks likely to grow. However, over recent years production has declined and internal consumption has grown within the region. The article suggests that politics may be an issue as some producers adopt a policy of resource nationalism and restrict foreign investment. It is also possible that supply not be as plentiful as thought.

10/00048 Latin America battles geology and politics to prevent decline in oil production; part 2 – regional survey and forecast

Anon., *Oil and Energy Trends*, 2009, 34, (7), 3–6.

Despite seemingly abundant reserves, Latin America faces challenges in meeting oil demand. Some reserves are heavy, bituminous crudes and extraction as liquid would require large inputs of capital and energy, other reserves lie in the deep waters of the Atlantic. An examination of the region by country suggests a number of obstacles to increasing production between now and 2015. Output may rise in only a handful of countries resulting in a decline for the continent as a whole and an even larger fall in net exports.

10/00049 Organic matter quality in reclaimed boreal forest soils following oil sands mining

Turcotte, I. *et al. Organic Geochemistry*, 2009, 40, (4), 510–519.

Following surface mining of the Athabasca Oil Sands deposits in northeastern Alberta, Canada, land reclamation entails the reconstruction of soil-like profiles using salvaged soil materials such as peat and mining by-products. The overall objective of this research was to assess soil organic matter (SOM) quality in different reclamation practices as compared to undisturbed soils found in the region. Soil samples (0–10 cm) were taken from 45 plots selected to represent undisturbed reference ecosites and reclamation treatments. Soil OM pools were isolated using a combination of acid hydrolysis and physical separation techniques. Chemical composition of the low density fractions was characterized using ramped cross polarization (RAMP-CP) ^{13}C nuclear magnetic resonance (NMR). Differences between disturbed and undisturbed sites reflected the influence of different botanical inputs (peat vs. forest litter) to SOM composition. Reconstructed soils were characterized by significantly lower alkyl over O-alkyl carbon (ALK/O-ALK) ratios (0.3) than undisturbed sites (0.5). For these reconstructed soils, a significantly higher proportion of soil carbon was present in the sand associated (Heavy sand) pool (49.2 vs. 37.3) and in the acid-unhydrolysable residue (AUR) fraction (61.3 vs. 54.7). These SOM parameters were significantly related to time since reconstruction, with the AUR (p value = 0.012) and Heavy sand (p value = 0.05) fractions decreasing with time since reconstruction, while the ALK/O-ALK ratio increased (p value = 0.006). These findings suggest that the ALK/O-ALK, AUR, and Heavy sand parameters are suitable indicators for monitoring SOM quality in these reconstructed soils following oil sands mining.

Derived liquid fuels

10/00050 Basic evidences for methanol-synthesis catalyst design

Arena, F. *et al. Catalysis Today*, 2009, 143, (1–2), 80–85.

A series of Cu–ZnO/ZrO_2 catalysts (Zn_{at}/Cu_{at}, 0–3; ZrO_2, 42–44 wt%) with markedly improved total (SA, 120–180 m^2/g) and metal surface area (MSA, 9–63 m^2/g) has been synthesized via the reverse co-precipitation under ultrasound field. Structure, adsorption properties and surface reactivity were probed by BET, XRD, TPR, N_2O-titration and TPD measurements of H_2, CO and CO_2, while the activity pattern in the CO_2 to CH_3OH hydrogenation reaction (T_R, 433–473 K; P_R, 1.0 MPa) has been addressed. An optimum ZnO loading (Zn_{at}/Cu_{at}, 0.3–0.8) ensures higher process productivity, while the apparent structure sensitive character of the title reaction relies on the synergism of metal hydrogenation and oxide basic sites (dual-site). The extent of the oxide/metal interface, probed by $Cu^{\delta+}/Cu_0$ and oxide-to-metal surface area (OSA/MSA) ratios, is the key-parameter allowing the normalization of the catalytic specific activity in a wide range (3–60%) of metal dispersion and the consequent structure insensitive character of the CO_2 hydrogenation reaction.

10/00051 Effect of the support acidity on the aromatic ring-opening of pyrolysis gasoline over Pt/HZSM-5 catalysts

Castaño, P. *et al. Catalysis Today*, 2009, 143, (1–2), 115–119.

This study evaluates the effect of the acidity of the support (HZSM-5) and the nature of the interaction between the active phases of the bifunctional Pt/HZSM-5 catalyst on the aromatic ring-opening of pyrolysis gasoline under hydrocracking conditions. The catalysts were characterized by N_2 adsorption–desorption isotherms, CO chemisorption, pyridine FTIR, NH_3 adsorption-DSC and NH_3 TPD. The catalyst screening in the pyrolysis gasoline hydrocracking demonstrated that: (i) the conversion of pyrolysis gasoline is linearly dependent on support acidity. At low acidities values the main mechanisms of ring-opening is through hydrogenolysis and thus, the less acidic catalyst shows higher conversion than expected; (ii) the synergysm between the metal and acid-sites is enhanced when using a bifunctional catalyst instead of a hybrid one, due to the increase in H_2 spill-over efficiency. However, in terms of activity, the most acid catalyst (hybrid) shows the highest aromatic conversion, in correspondence with (i).

10/00052 Fe and Pt carbon nanotubes for the electrocatalytic conversion of carbon dioxide to oxygenates

Gangeri, M. *et al. Catalysis Today*, 2009, 143, (1–2), 57–63.

Using Pt/CNT or Fe/CNT electrocatalysts it is possible to convert carbon dioxide to liquid fuels, particularly isopropanol. Fe/CNT shows a better behaviour than Pt/CNT, although a faster deactivation. The main reason for deactivation is cross-over of the electrolyte, particularly of K ions. They react with iron particles and cause their dissolution and migration. In the case of Pt/CNT there is no, or minor, dissolution of metal, but potassium covers the Pt particles and/or induce deactivation. It is shown, however, that the electrolyte was necessary to simulate the half-cell of the full photoelectrocatalytic device, while in the latter no electrolyte is needed, being the protons and electrons produced by water splitting. The elimination of the electrolyte probably could eliminate or significantly reduce a main cause determining the observed fast deactivation.

10/00053 Hydrogenation of heavy liquids from a direct coal liquefaction residue for improved oil yield

Li, J. *et al. Fuel Processing Technology*, 2009, 90, (4), 490–495.

For hydrogenation of heavy liquids in direct coal liquefaction residue (DCLR) within the direct coal liquefaction (DCL) process, heavy liquids in a DCLR derived from a bench-scale Shenhua DCL process using Shenhua coal are evaluated under two conditions. One simulates the coal liquefaction conditions of the Shenhua plant in the presence of a Fe-based Shenhua catalyst; the other one simulates the online hydrotreating conditions in the presence of a $NiMo/Al_2O_3$ catalyst. The results show that the heavy liquids of DCLR can be hydrogenated under these two conditions yielding less heavy products; hydrogenating the heavy liquids under the online hydrotreating conditions is more effective than that under the coal liquefaction conditions; the preasphaltene fraction is a main problem that yields non-soluble materials under these hydrogenation conditions. The results suggest that hydrogenation of toluene soluble and tetrahydrofuran soluble fractions of the DCLR under the coal liquefaction and online hydrotreating conditions is feasible, but their conversion to lighter products are not apparent under the coal liquefaction conditions, and elimination of the formation of tetrahydrofuran insoluble fraction in the online hydrotreator should be considered.

10/00054 Hydroisomerization and hydrocracking of hydrocracker bottom for producing lube base oil

Ling, H. *et al. Fuel Processing Technology*, 2009, 90, (4), 531–535.

The reaction of hydrocracker bottom hydroisomerization and hydrocracking was studied in a fixed bed micro reactor over a commercial catalyst. Normal hexadecane was used as the model compound to judge the reactivity of the catalyst. Then, the hydrocracker bottom was investigated, and the reaction liquid products were collected and distilled into light and heavy fractions for detailed investigation. Their hydrocarbon types and carbon number distribution were fully analysed. Results indicate that normal paraffins can easily be hydroconverted into isoparaffins or small molecules. Isoparaffins and monocycloalkanes have similar hydroisomerization and hydrocracking properties. Fused cycloalkanes are hard to be cracked. Hydroconversion of normal paraffins, isoparaffins and monocycloalkanes dominate the reason of the drop of VI and pour point.

10/00055 Isobaric vapor–liquid–liquid equilibrium and vapor–liquid equilibrium for the system water–ethanol-1,4-dimethylbenzene at 101.3 kPa

Gomis, V. *et al. Fluid Phase Equilibria*, 2009, 281, (1), 1–4.

An all-glass, dynamic recirculating still equipped with an ultrasonic homogenizer has been used to determine vapour–liquid (VLE) and vapour–liquid–liquid (VLLE) equilibria. Consistent data have been obtained for the ternary water + ethanol + *p*-xylene system at 101.3 kPa for temperatures in the range of 351.16–365.40 K. Experimental results have been used to check the accuracy of the UNIFAC, UNIQUAC and NRTL models in the liquid–liquid region of importance in the dehydration of ethanol by azeotropic distillation.

10/00056 Liquefaction of rice straw in sub- and supercritical 1,4-dioxane–water mixture

Li, H. *et al. Fuel Processing Technology*, 2009, 90, (5), 657–663.

The critical liquefaction of rice straw in sub- and supercritical 1,4-dioxane–water mixture was investigated in a 500 mL autoclave at a temperature of 260–340 °C, resistance time of 0–20 min, and volume ratios 0–100 vol.% (1,4-dioxane:mixture). The yields of oil and PA + A (preasphaltene and asphaltene) were in the range of 29.64–57.30 wt% and 6.42–22.68 wt%, depending on the temperature, resistance time and volume ratio. The synergistic capability of 1,4-dioxane–water mixture could allow the great decomposition of the tubular structure of lignocelluloses. It was shown by the results that the 'oxygen-transfer' reaction, deoxygenation and decarboxylation may occur in the liquefaction of rice straw with 1,4-dioxane–water mixture, while deoxygenation and decarboxylation may be the main reaction. The oil and PA + A fractions obtained at different volume ratios were analysed by FTIR and GC–MS to investigate the effect of the ratios on the type of the compounds in the liquid products. It is shown that the nucleophilic and hydrolytic functions of water might be weaken at the higher ratio of 1,4-dioxane runs, resulting the lower amount of phenolic, acidic, hydrocarbon and ester derivatives in the oil and PA + A fractions.

10/00057 $NiO–W_2O_3/Al_2O_3$ catalysts for the production of ecological gasoline: effect of both NiO and the preparation method on the isobutene oligomerization selectivity

Tzompantzi, F. *et al. Catalysis Today*, 2009, 143, (1–2), 132–136.

The results obtained for the oligomerization of C_4 olefins in order to produce high octane ecological gasoline by using $NiO–W_2O_3/Al_2O_3$ catalysts prepared by both the wetness impregnation and sol–gel methods, are reported. High selectivity towards $C_8^=$ olefins, avoiding the formation of heavier olefinic products, as well as an excellent stability were reached by means of the $NiO–W_2O_3/Al_2O_3$ impregnated catalyst. The characterization of the catalysts by XRD, total specific surface area and FTIR pyridine adsorption are also reported.

10/00058 Performance of Euro III common rail heavy duty diesel engine fueled with gas to liquid

Wang, H. *et al. Applied Energy*, 2009, 86, (10), 2257–2261.

The effect of synthetic diesel fuel made from natural gas (gas to liquid, GTL) on the engine performances (such as power, efficiency and emission) was carried out on one Euro III common rail heavy duty diesel engine without any modification. The results showed that the engine fuelled with GTL had some variations compared with the one fuelled with petroleum-based low sulfur diesel fuel (sulfur content less 50 ppm). The maximum torque and power were decreased by 1.3% and 1.9%, respectively. The specific fuel consumption increased in volume but had no change in mass. Under the load characteristics, the NO_x, CO and THC were reduced by 13%, 55% and 55%, respectively. During the ESC cycle test, the NO_x, CO, THC and PM were reduced by 5.2%, 19.3%, 19.8% and 33%, respectively.

10/00059 Thermoeconomic analysis of a large industrial propane refrigeration cycle used in NGL recovery plant

Mehrpooya, M. *et al. International Journal of Energy Research*, 2009, 33, (11), 960–977.

In this paper a propane refrigeration cycle has been analysed by thermoeconomic approach. This cycle is used for obtaining required refrigeration in a natural gas liquids (NGL) recovery plant. Most of the advanced methods in thermoeconomic diagnosis are examined on power plants. In this work thermoeconomic diagnosis is applied to NGL recovery plant. The impact of the component inefficiencies on the fuel plant consumption, and the effect of a component inefficiency (intrinsic malfunction) on the rest of the plant components (induced malfunctions and dysfunctions), are analysed and quantified. The results show that thermoeconomics is not only a diagnostic tool, but also a useful tool for optimization, which can be applied to complex refrigeration processes in NGL recovery plants.

03 GASEOUS FUELS

Sources, properties, recovery, treatment

10/00060 A method to predict geomechanical properties and model well stability in horizontal boreholes

Gentzis, T. *et al. International Journal of Coal Geology*, 2009, 78, (2), 149–160.

A methodology is proposed to quickly assess the stability risk for horizontal wells drilled in coal seams. The first task involves the estimation of strength and deformation parameters of the coal by indirect methods, such as the use of core description to assign a Geological Strength Index (GSI). The second task involves the use of a finite element analysis called FLAC to investigate factors such as the depth of fluid penetration while drilling the horizontal well and the stability of the wellbore during simulated production. These two factors are important because coal fines generated by the drill bit action are carried by the drilling fluid into the cleat system of the coal, thereby plugging the permeability pathways, and causing formation damage. On the other hand, a wellbore that may become unstable during pressure drawdown would require a perforated or slotted production liner. In this study, the conditions of drilling and production necessary for a stable horizontal well drilled into a Mannville coal seam at 750–800 m in the central Alberta Plains, were studied. Modelling showed that the depth of fluid penetration would be at least 2.2 m if there is no filter cake formation while drilling underbalanced. Drilling fluid penetration would be minimal if a filter cake is formed under overbalanced conditions. Furthermore, FLAC analysis showed that drilling a smaller diameter hole (5 cm) would be preferable because this size results in a stable wellbore during production compared to the standard 15-cm diameter hole.

10/00061 Distribution of thermogenic methane in Carboniferous coal seams of the Donets Basin (Ukraine): ‘Applications to exploitation of methane and forecast of mining hazards’

Alsaab, D. *et al. International Journal of Coal Geology*, 2009, 78, (1), 27–37.

The main purpose of this contribution is to estimate methane production and to define its migration paths and storage in the Donets Basin formations for exploitation of methane and forecast of mining hazards. In order to study methane migration and storage, maps of production calculated by 2D modelling, adsorption capacity of methane in coal, and present-day methane contents were constructed for an altitude of –300 m (close to 500 m depth) in this basin. The results show that three principal factors influenced the methane migration and accumulation in Donets Basin: (1) faults that acted as migration pathways, (2) a replacement of thermogenic methane by endogenic CO_2 in the central and SE parts, and (3) the occurrence of magmatic events in some areas in this basin. Finally, in Donbas, the areas with the highest methane potential and the maximum risk of outburst are not the areas with anthracite that produce the highest volume of methane, but areas with volatile bituminous coals where an impermeable cover preserved the accumulated gas until the Cenozoic and where dextral shear belts facilitated its migration.

10/00062 Liquid piston gas compression

Van de Ven, J. D. and Li, P. Y. *Applied Energy*, 2009, 86, (10), 2183–2191.

A liquid piston concept is proposed to improve the efficiency of gas compression and expansion. Because a liquid can conform to an irregular chamber volume, the surface area to volume ratio in the gas chamber can be maximized using a liquid piston. This creates near-isothermal operation, which minimizes energy lost to heat generation. A liquid piston eliminates gas leakage and replaces sliding seal friction with viscous friction. The liquid can also be used as a medium to carry heat into and out of the compression chamber. A simulation is presented of the heat transfer and frictional forces for a reciprocating piston and a liquid piston. In the application of an air compressor, with a pressure ratio of 9.5:1 and a cycle frequency of 20 Hz, the liquid piston decreased the energy consumption by 19% over the reciprocating piston. The liquid piston and the reciprocating piston exhibited a total efficiency of 83% and 70% respectively. The liquid piston demonstrated significant improvements in the total compression efficiency in comparison to a conventional reciprocating piston. This gain in efficiency was accomplished through increasing the heat transfer during the gas compression by increasing the surface area to volume ratio in the compression chamber.

10/00063 Petrographic properties of major coal seams in Turkey and their formation

Toprak, S. *International Journal of Coal Geology*, 2009, 78, (4), 263–275.

Most types of coal in Turkey are generally low in rank: lignite, and subbituminous. Most of the coal was formed during the Miocene, Eocene, and Pliocene ages. There are only a few thin Jurassic-age coal occurrences in Turkey. Pennsylvanian age bituminous coal is found on the Black Sea coast. General implications of the petrographic properties of Turkey’s coal seams and coal deposits have not yet been taken into consideration comparatively or as a whole. For this study, about 190 channel samples were collected from different locales. The composite profile samples of the seams were taken into considerations. The content and depositional properties as well as some chemical and physical properties of the main coal seams are compared. All coal samples tend to have similar coal petrographic properties and were deposited in intermontane lacustrine basins. Later, they were affected by faulting and post-depositional volcanic activity. As a result, there are variations in the properties and rank of the coal samples. The most abundant coal maceral group is huminite and the most abundant maceral is gelinite. The liptinite and inertinite contents of the coal are low and the maceral contents of the coals show great similarity. The depositional environments of the all coals are lacustrine dominated.

10/00064 Preliminary evaluation of the coalbed methane production potential and its geological controls in the Weibei Coalfield, Southeastern Ordos Basin, China

Yao, Y. *et al. International Journal of Coal Geology*, 2009, 78, (1), 1–15.

This study considers the coalbed methane (CBM) geology, resource and production potential in the Weibei Coalfield, southeastern Ordos Basin based on geological surveys and laboratory measurements. The results showed that coal rank varies both laterally and vertically and changes from volatile bituminous coals in the margin to anthracites towards the basin (1.6–2.5% R_o). Coals are composed of 60–85% vitrinite, 15–40% inertinite and a trace amount of minerals. Methane isothermal adsorption measurements of 20 coal samples revealed that the maximum adsorption capacity (on a dry and ash-free basis) of coals, which are affected by coal rank, coal maceral, coal lithotype and especially to the moisture content, varies from 13.91 to 29.54 m^3/t. Estimated gas contents range from 0 to 15 m^3/t. These data yield an estimated in-place CBM resource of 2.5×10^{11} m^3 for the Weibei Coalfield. In combination with the geological information, the data indicated that the tectonic evolution of the basin had important influences on gas accumulation, preservation, and escaping. Particularly, Late Cretaceous extensional faults may have served as the escaping conduits for gas and thus resulted in the low gas content and low gas saturation in the western area of the Weibei Coalfield. The permeability is between 0.1 and 10 mD and the porosity ranges from 2 to 7%. Petrologic permeability analyses revealed that the permeability is mainly related to the endo-microfractures, porosity and mineralization of coals. Finally, based on the mathematic analytic hierarchy process and the evaluated factors including coal thickness, gas content, coal rank, CBM resource concentration, permeability and porosity, burial depth and tectonic type, the best prospective target area for CBM production is forecasted to be west of the Sangshuping mine and circumjacent to the Xuefeng deep district in the central part of the Hancheng coal district.

10/00065 Reservoir rock properties of coal measure strata of the Lower Monongahela Group, Greene County (Southwestern Pennsylvania), from methane control and production perspectives

Karacan, C. Ö. *International Journal of Coal Geology*, 2009, 78, (1), 47–64.

The methane emission rate into an underground mine environment from overburden strata during longwall mining is impacted by reservoir and geomechanical characteristics of the coal measure rocks in the overlying strata, as well as the presence of any coal seam. The reservoir characteristics and how they change during mining potentially affect the performance of gob gas ventholes, which consequently impact the efficiency of methane control in the mining environment. This study presents reservoir and elastic properties of coal measure rocks in the Lower Monongahela Group in Greene County, southwestern Pennsylvania, of the Northern Appalachian Basin. Since the source of methane in this region from underground mining is located between the Sewickley coal and the Pittsburgh coal, a specific emphasis was given to this interval. Core analyses were performed in the laboratory to determine rock porosity and permeability. Geophysical logging data (gamma, density, sonic) obtained from two exploration boreholes were used for evaluating formation boundaries, shale contents, log porosities, and geomechanical properties of formations. Permeability was also calculated using density-log data and empirical equations and compared with laboratory measurements and slug tests performed in isolated intervals of boreholes. The results presented in this study can be used as data sources for reservoir studies related to the production and control of methane.

10/00066 Terrestrial methane seeps and mud volcanoes: a global perspective of gas origin

Etiope, G. *et al. Marine and Petroleum Geology*, 2009, 26, (3), 333–344.
A global database of gas composition and methane stable isotopes of 143 terrestrial mud volcanoes from 12 countries and 60 seeps independent from mud volcanism from eight countries, was compiled and examined in order to provide the first worldwide statistics on the origin of methane seeping at the earth's surface. Sixteen seep data were coupled with their associated subsurface reservoirs. The surface seepage data indicate that at least 76% of the mud volcanoes release thermogenic gas, with only 4% biogenic and 20% with mixed character. The average (201 data) of methane concentration and methane carbon isotope ratios ($\delta^{13}C_1$) of mud volcanoes are 90% v/v and −46.4‰, respectively. The other types of seeps, which are independent from mud volcanism, have an average $\delta^{13}C_1$ value that is slightly higher (−42.9‰). Gases from mud volcanoes are generally lighter (more methane, less ethane and propane) than their associated reservoir gases, suggesting a molecular fractionation during advective fluid migration. Other types of seeps, especially 'dry' seeps, maintain the reservoir $C_1/(C_2+C_3)$ 'Bernard' ratio. Mud volcanoes behave like a 'natural refinery' and the origin of gas more isotopically enriched than −50‰ and with $C_1/(C_2+C_3)>500$ should be attributed to a thermogenic source, rather than partial oxidation of biogenic gas. Some data that appear biogenic in the 'Bernard diagram' can be explained by molecular fractionation of mixed gas. Consequently, the 'Bernard' parameter may be misleading when applied to mud volcanoes since it does not always reflect the original gas composition. The mechanisms of the molecular advective segregation should be studied quantitatively by specific models and experiments.

10/00067 Warm water flooding of confined gas hydrate reservoirs

Phirani, J. and Mohanty, K. K. *Chemical Engineering Science*, 2009, 64, (10), 2361–2369.
Large quantities of natural gas hydrate are present in marine sediments along the coastlines of many countries as well as in arctic regions. This research is aimed at assessing techniques to produce natural gas from marine hydrate deposits. A multiphase, multicomponent, thermal, 3D simulator is used, which can simulate production of hydrates both in equilibrium and kinetic modes. Three components (hydrate, methane, and water) and four phases (hydrate, gas, aqueous-phase, and ice) are considered in the simulator. This work simulates warm water flooding and depressurization for hydrate production from a confined reservoir with a hydrate layer underlain by a water layer. Water flooding has been studied as a function of injection temperature, injection pressure and production pressure. For high injection temperature and high production pressure, warm water injection is preferred over depressurization; an increase in injection pressure increases the heat influx to the reservoir making the gas production faster. If a low pressure can be maintained at the production well or the injection temperature is not high, then just depressurization is the best method of production. As reservoir porosity and permeability increase and the heat transfer coefficient to the over- and under-burden decreases, the warm water injection process becomes more favorable.

Transport, storage

10/00068 A generalized correlation for predicting gas–condensate relative permeability at near wellbore conditions

Jamiolahmady, M. *et al. Journal of Petroleum Science and Engineering*, 2009, 66, (3–4), 98–110.
This paper presents a generalized correlation based on relative-permeability-ratio, which is closely related to a fractional flow of gas and condensate. The parameters of the new correlation are either universal, applicable to all types of rocks, or can be determined from commonly measured petrophysical data. The performance of the correlation has been evaluated over a relatively wide range of interfacial tension (IFT) and velocity variations. This has been conducted by comparing its prediction with the gas–condensate relative permeability values measured on porous media with very different characteristics. These data had not been used in developing the correlation. The results are quite satisfactory confirming the generality of the correlation in providing reliable information on gas–condensate relative permeability values for near wellbore conditions.

10/00069 Application of crosswell seismic tomography using difference analysis with data normalization to monitor CO_2 flooding in an aquifer

Onishi, K. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (3), 311–321.
A pilot-scale experiment for carbon dioxide (CO_2) sequestration was undertaken at the Nagaoka test field in Japan. Time-lapse crosswell seismic tomography was conducted to detect and monitor the movement of CO_2 injected into an aquifer. The authors applied difference analysis with data normalization (DADN) to the time-lapse data to eliminate false images that were apparent in a conventionally processed difference section. Conventional difference analysis calculates travel-time delays after inversion, whereas the DADN method calculates them from raw travel-time records before inversion. Thus, fewer errors are generated with the DADN method compared to a conventional inversion analysis. The authors also applied the DADN method to time-lapse tomography data recorded before and after the injection of CO_2 and computed the velocity variation in a subsurface section, which clearly showed the distribution of CO_2 flooding within a high permeability zone in the aquifer and showed no CO_2 leakage into the caprock. The results also show the maximum velocity decrease as a result of CO_2 injection was about 9%, which is close to the results obtained in laboratory experiments. Finally, numerical simulations were inverted to test the effectiveness of the conventional and DADN methods in dealing with noise. These tests showed that the DADN method effectively reduces unique coherent noise for particular receiver and source combinations. It was concluded that the DADN method provides useful data for monitoring the flow of CO_2 sequestered in underground aquifers.

10/00070 Fracture analysis of hydrogen storage composite cylinders with liner crack accounting for autofrettage effect

Hu, J. and Chandrashekhara, K. *International Journal of Hydrogen Energy*, 2009, 34, (8), 3425–3435.
An understanding of fracture behaviour is crucial to the safe installation and operation of high-pressure composite cylinders for hydrogen storage. This work has developed a comprehensive finite element model to investigate axial surface flaws in cylinder liners using the fracture mechanics and a global–local finite element technique. Since the autofrettage process has a strong influence on cylinder fracture behaviour, it is also considered in this analysis. The simulation process is broken down into three steps in order to precisely extract fracture parameters and incorporate the autofrettage effect. In the first step, the global model performs the autofrettage simulation to study the residual stress with consideration of both material hardening and the Bauschinger effect. In the second step, the global model uses residual stress to compute displacement for the local model. Finally, in the third step, the local model extracts the values of stress intensity factor and J-integral. Comparison is conducted on the fracture parameters with various autofrettage levels and crack shapes. The vicinity of the crack front is also studied by the size and shape of the plastic zone, and the validity of stress intensity factor and J-integral dominances is examined.

10/00071 Methodology to improve the lifetime of type III HP tank with a steel liner

Comond, O. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 3077–3090.
The present paper aims at studying a high-pressure hydrogen storage vessel, combining a steel liner and a wrapped composite reinforcement. Nowadays, this means of storage is notably used in transport. However, limits appear insofar as fatigue problem happens when the operating pressure is 700 bar. This matter has to be solved. This study tries to arrange a method to build a 700 bar vessel which could resist to cyclic pressure loading, and particularly focuses on the behaviour of the liner which seems to be the critical element to control. In addition, as a large part of this gaseous storage is bound to be on board, the composite optimization and thus weight optimization is considered.

10/00072 Numerical simulations on the influence of matrix diffusion to carbon sequestration in double porosity fissured aquifers

Carneiro, J. F. *International Journal of Greenhouse Gas Control*, 2009, 3, (4), 431–443.
The double porosity model for fissured rocks, such as limestones and dolomites, has some features that may be relevant for carbon sequestration. Numerical simulations were conducted to study the influence of matrix diffusion on the trapping mechanisms relevant for the long-term fate of CO_2 injected in fissured rocks. The simulations show that, due to molecular diffusion of CO_2 into the rock matrix, dissolution trapping and hydrodynamic trapping are more effective in double porosity aquifers than in an equivalent porous media. Mineral trapping, although assessed indirectly, is also probably more relevant in double porosity aquifers due to the larger contact surface and longer contact time between dissolved CO_2 and rock minerals. However,

stratigraphic/structural trapping is less efficient in double porosity media, because at short times CO_2 is stored only in the fissures, requiring large aquifer volumes and increasing the risk associated to the occurrence of imperfections in the cap-rock through which leakage can occur. This increased risk is also a reality when considering storage in aquifers with a regional flow gradient, since the CO_2 free-phase will move faster due to the higher flow velocities in fissured media and discharge zones may be reached sooner.

10/00073 TMGAS: a new TOUGH2 EOS module for the numerical simulation of gas mixtures injection in geological structures

Battistelli, A. and Marcolini, M. *International Journal of Greenhouse Gas Control*, 2009, 3, (4), 481–493.

Injection of gas mixtures in geological structures is performed for a variety of different purposes including natural gas storage operations, CO_2 flooding and water alternate gas injection for enhanced oil recovery, and more recently for the sequestration of greenhouse gases and the disposal of acid gases produced by sour hydrocarbon reservoirs. The injection of multi-component mixtures into saline aquifers and hydrocarbon reservoirs requires the understanding of the processes that govern the performances of injection wells, the fluid migration within the reservoirs, and the possible recovery of additional hydrocarbon reserves. Conventional compositional simulators employed by the oil industry, while implementing complex phase equilibrium algorithms for the hydrocarbon phases, often give only an approximate description of the aqueous phase behaviour and properties. In particular, the injection of mixtures mainly composed by acid gases such as CO_2 and H_2S drives pronounced modifications of aqueous phase chemical equilibria promoting water–rock reactions with possible alteration of reservoir and cap rock, as well as of wellbore cement sheaths. The gas mixtures usually injected in undersaturated conditions with respect to water, progressively vaporize the aqueous phase, concentrating the dissolved solids until they precipitate as new mineral phases, eventually reducing the initial rock porosity and permeability. Vaporized water is transported further from the injection wellbore to possibly condense again in the presence of proper thermodynamical conditions. TMGAS, a new Equation of State module for the TOUGH2 reservoir simulator, has been developed to model the injection of mixtures of inorganic gases and hydrocarbons in geological structures at conditions conventionally found in deep sedimentary basins.

Economics, business, marketing, policy

10/00074 Assessment of primary impacts of a hydrogen economy in New Zealand using UniSyD

Leaver, J. D. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 2855–2865.

Small economies such as New Zealand risk significant economic hardship without careful evaluation of alternatives to petroleum-based transportation due to the adverse effects of climate change and depleting international oil reserves. This paper uses an integrated multi-regional multi-fleet system dynamics model of New Zealand's energy economy to assess the primary impacts of alternative vehicle fleet technologies. Results suggest that hydrogen-fuelled internal combustion engine vehicles (HICEs) and fuel cell vehicles (FCVs) may offer significantly greater economic savings than battery electric vehicles (BEVs) due to a much lower capital cost. Under the base case used, 65% of the light fleet are HICEs and FCVs and 5% BEVs. Excluding hydrogen vehicles from the vehicle fleet can result in an average annual cost of US$562 per vehicle between 2015 and 2050. Co-production of hydrogen and electricity using coal gasification with carbon capture and storage is the dominant long term hydrogen production technology.

10/00075 Bangladesh faces gas and power shortages

Anon., *Oil and Energy Trends*, 2009, 34, (6), 7–8.

Bangladesh is struggling to cope with increasing shortages of gas and electricity. The government's energy policy has been based on meeting the rise in power demand by building more generating stations to run on domestically produced gas; but gas production is not growing quickly enough. The government's response has been to order the national oil and gas company, Petrobangla, to divert gas supplies from heavy industry to the power generators; but even this has failed to release enough gas to meet the country's demand for electricity. Bangladesh is now trying to import gas but this is proving difficult as well.

10/00076 Evaluation of soil biological activity after a diesel fuel spill

Serrano, A. *et al. Science of the Total Environment*, 2009, 407, (13), 4056–4061.

Diesel fuel contamination in soils may be toxic to soil microorganisms and plants and acts as a source of groundwater contamination. The objective of this study was to evaluate the soil biological activity and phytotoxicity to garden cress (*Lepidium sativum* L.) in a soil polluted with diesel fuel. For this, a diesel fuel spill was simulated on agricultural soil at dose $1\,l\,m^{-2}$. During the experiment (400 days) the soil was not covered in vegetation and no agricultural tasks were carried out. A stress period of 18 days following the spill led to a decrease in soil biological activity, reflected by the soil microbial biomass and soil enzymatic activities, after which it increased again. The n-C_{17}/Pristine and n-C_{18}/Phytane ratios were correlated negatively and significantly with the dehydrogenase, arylsulfatase, protease, phosphatase and urease activities and with the soil microbial biomass during the course of the experiment. The β-glucosidase activity indicated no significant connection with the parameters related with the evolution of hydrocarbons in the soil. Finally, the germination activity of the soil was seen to recover 200 days after the spill.

10/00077 Households' willingness to pay for safeguarding security of natural gas supply in electricity generation

Damigos, D. *et al. Energy Policy*, 2009, 37, (5), 2008–2017.

Security of energy supply is a major issue for all EU Member States due to Europe's increasing dependence on imported fossil-fuel sources and the continuous rise in energy demand. The latter is of particular importance in electricity sector given the continuously increasing use of gas for electricity generation. In order to properly tackle with the problem, concerted actions are required by the EU Member States in several levels, i.e. legislative, political, etc. Nevertheless, these actions will come at an additional cost paid by the society either through increased electricity bills or through public financing for energy security investments. Thus, such policies should be justified on the basis of cost-benefit analysis. Towards this direction, it may be necessary to take into account non-market costs and benefits, i.e. the value that consumers place on interruptions avoided. In order to explore households' perceptions and willingness to pay for securing gas supply for electricity production, an empirical study was conducted by means of the contingent valuation method. The results indicate that consumers are willing to pay a premium on their electricity bills in order to internalize the external costs of electricity production, in terms of energy security, which are caused from imported fuels.

10/00078 Numerical simulation of stress distributions and displacements around an entry roadway with igneous intrusion and potential sources of seam gas emission of the Barapukuria coal mine, NW Bangladesh

Islam, M. R. and Shinjo, S. J. *International Journal of Coal Geology*, 2009, 78, (4), 249–262.

This paper uses two-dimensional boundary element method (BEM) numerical modelling to analyse the deformation and failure behaviour of a coal seam and to understand the nature of gas flow into a roadway entering the Barapukuria coal mine in Bangladesh. The Barapukuria basin contains Permian-aged Gondwana coals with high volatile B bituminous rank. Three models (A, B, and C) are presented here. Model A assumes horseshoe-shaped geometry, model B assumes trapezoid-shaped geometry, and model C assumes horseshoe-shaped geometry coupled with a roof fall-induced cave generated by the break-up of rock materials along the vertical dimension of an igneous dyke. The simulation results show that there is little difference in strata deformation between models A and B. In model A, there is no horizontal tensional stress and the overall horizontal stress patterns are compressive, while the distribution and magnitude of vertical stress show higher tensional stresses on the immediate rib sides and floor. In model B, both horizontal and vertical stress distributions indicate low to medium tensional stresses on the immediate roof, floor, and rib sides, but compressive stresses are prominent toward the interior of the coal seam. Deformation vectors indicate that failure extends laterally to about 7.5 m around the excavation geometry. On the contrary, for model C, the distributions and magnitudes of horizontal and vertical stress show higher tensional stresses in both rib sides of the roof fall zone. The deformation around the dyke-induced perturbation zone affects a large volume of coal. The deformation vectors with high magnitudes are nearly horizontal and propagate laterally up to 30 m; whereas, low-magnitude deformation vectors extend about 25 m toward the roof and 20 m toward the floor. The vertical tensional displacement, which is concentrated in the floor and the left and right hand sides of the roof, propagates about 30 m on both sides and about 22 m in the floor. From these simulation results, it is thought that the extension of the dyke-induced perturbation zone toward the roof, floor, and rib sides of the entry roadway initially creates small tensional cracks that gradually grow into large-scale tensional features. These features could also be responsible for high concentrations of gas, which are emitted into the mine from fractured coals due to insufficient mine ventilation and low atmospheric pressure.

Derived gaseous fuels

10/00079 A comparison of basket willow and coal hydrogasification and pyrolysis

Porada, S. *Fuel Processing Technology*, 2009, 90, (5), 717–721.

The study investigated the course of basket willow hydrogasification and comparing that process to the hydrogasification of bituminous coal. The examinations focussed on basket willow (*Salix viminalis*), bituminous coal of low degree of metamorphism and their blends at the mass ratio 1:1. Measurements of evolution kinetics of gaseous hydrocarbons during hydrogasification of those materials were conducted in the atmosphere of hydrogen under the pressure of 2.5 MPa. In the investigations, the non-isothermal method was employed. The examined samples were heated from ambient temperature up to 1200 K at the rate of 3 K/min. The highest yields of the examined products were recorded during hydrogasification of coal, and the lowest yield was observed in the process involving the use of basket willow. For comparison, measurements of basket willow pyrolysis were also conducted. It was established that in the process of hydrogasification, even at a relatively low pressure which was used in the examinations, it is possible to achieve the yield and conversion ratios of C to the hydrocarbons C_1–C_3 which are approximately five times higher than in the case of pyrolysis conducted in the atmosphere of an inert gas.

10/00080 Air–steam gasification of biomass in a fluidised bed: process optimisation by enriched air

Campoy, M. *et al. Fuel Processing Technology*, 2009, 90, (5), 677–685.

The effect of oxygen concentration in the gasification agent was studied by enriched-air–steam biomass gasification tests in a bubbling fluidized-bed gasification (FBG) plant. The oxygen content in the enriched air was varied from 21% (v/v, i.e. air) to 40% (v/v), aiming at simulating FBG where enriched air is produced by membranes. The stoichiometric ratio (ratio of actual to stoichiometric oxygen flow rates) and steam-to-biomass ratio (ratio of steam to biomass, dry and ash-free, flow rates) were varied from 0.24 to 0.38 and from 0 to 0.63, respectively. The tests were conducted under simulated adiabatic and autothermal conditions, to reproduce the behaviour of larger industrial FBG. The temperature of the inlet gasification mixture was fixed consistently at 400 °C for all tests, a value that can be achieved by energy recovery from the off-gas in large FBG without tar condensation. It was shown that the enrichment of air from 21 to 40% v/v made it possible to increase the gasification efficiency from 54% to 68% and the lower heating value of the gas from 5 to 9.3 MJ/Nm^3, while reaching a maximum carbon conversion of 97%. The best conditions were found at intermediate values of steam-to-biomass ratio, specifically within the range 0.25–0.35. The enriched-air–steam gasification concept explored in this work seems to be an interesting option for the improvement of standalone direct air–blown FBG because it considerably improves the process efficiency while maintaining the costs relatively low as compared to oxygen-steam gasification.

10/00081 Calcium oxide for CO_2 capture: operational window and efficiency penalty in sorption-enhanced steam methane reforming

Solieman, A. A. A. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (4), 393–400.

Calcium oxide (CaO) is a material that is being widely investigated in the context of CO_2 capture. One such application is as a CO_2 sorbent in the sorption-enhanced steam methane reforming processes (SERP). CO_2 is captured in an adsorption mode, where the conversion of CH_4 to H_2 is also enhanced, and released later in a separate desorption mode. This work presents an analysis of the relation between different process conditions and parameters during both adsorption and desorption modes. The interrelation between these conditions and the sorbent properties as well as the targeted carbon capture ratio is analysed. Conditions relevant for capturing 85% of carbon in the feed on CaO are determined and interlinked. A steam-to-carbon ratio of 4.2 has been determined to be relevant under 600 °C and 17 bar adsorption conditions. Similarly, process conditions relevant for regenerating the sorbent are determined and interlinked. For purge steam-to-CO_2 ratio of 1.8 at a desorption pressure of 1 bar, relevant desorption temperature has been calculated to be 820 °C. System simulations under these adsorption and desorption conditions resulted in a system efficiency of 50.8%. Effect of tuning process operating conditions on system efficiency as well as the efficiency penalty associated with the regeneration of the sorbent are investigated by process simulations using Aspen Plus®. Possible system heat integration routes to reduce the efficiency penalty are proposed and the results of the process simulations are presented.

10/00082 Exergetic evaluation and improvement of biomass-to-synthetic natural gas conversion

Juraík, M. *et al. Energy Environmental Science*, 2009, 2, (7), 791–801.

Synthetic natural gas (SNG) is suggested as an important future energy carrier. The conventional route for SNG production is based on gasification of biomass to synthetic gas and the subsequent methanation of synthetic gas to SNG. This study is aimed to analyse the process units using the concept of exergy. Exergy analysis is a promising method, based on the 2nd law of thermodynamics, to analyse and improve chemical processes. In this work a detailed exergy analysis is performed for the SNG process based on woody biomass gasification. The main elements of the system are gasifier, gas cleaning, synthetic gas compression, methanation and final SNG condition. The above-mentioned process was simulated with a computer model using the flow-sheeting program Aspen Plus. Optimal values of the process conditions, particularly for the methanation reactors, are found. The internal exergy losses of different system units are evaluated. The largest internal exergy losses take place in the gasifier, methanation section and CO_2 capture unit. The highest overall exergetic efficiency of 72.6% was found applying the following operating conditions: gasifier 700 °C and 1 bar; 1st methanation reactor 580 °C and 2nd methanation reactor 405 °C.

10/00083 Fischer Tropsch reaction from a mixture similar to biosyngas. Influence of promoters on surface and catalytic properties of Co/SiO_2 catalysts

Escalona, N. *et al. Catalysis Today*, 2009, 143, (1–2), 76–79.

A Fische–Tropsch reaction using a mixture similar to that obtained from biomass transformation (biosyngas) has been studied on promoted Co/SiO_2 catalysts. As promoters, Cu, Zn, Re and Ru at two different amounts were analysed. The promoter affects both the reducibility and the dispersion of Co species, which have an important effect in the activity and selectivity of the studied catalysts. Re and Ru significantly increase both the activity and the selectivity to long-chain hydrocarbons, whereas in those promoted by Cu and Zn the effect is strongly affected by the amount of promoter. In those with higher amount of promoter (0.5 wt%), the formation of surface spinels or the blocking of the Co active sites by the copper itself produces a drop in the catalytic activity. The product distribution of the liquid extract reveals the presence of hydrocarbons from C_6 to higher than C_{14+}, in most of the catalysts.

10/00084 Hydrogen production from coal using coal direct chemical looping and syngas chemical looping combustion systems: Assessment of system operation and resource requirements

Gnanapragasam, N. V. *et al. International Journal of Hydrogen Energy*, 2009, 34, (6), 2606–2615.

Coal direct chemical looping (CDCL) substitutes the gasification process in syngas chemical looping (SCL), thus eliminating the need for higher oxygen consumption. In this study, operating conditions are assessed for CDCL and SCL, directed towards hydrogen production from coal. The main objective is to increase the overall H_2/CO_2 ratio for a given amount of coal, based on the various conditions. The operating variables considered to be part of a resource optimization analysis include: (i) inlet conditions to the primary reactors, (ii) minimum resource requirements (air, steam and iron oxide), (iii) hydrogen-to-component ratios, and (iv) effect of coal carrier gas. The results suggest that CDCL has a higher hydrogen-to-CO_2 ratio than SCL along with advantages such as low overall resource requirements (steam and air) and fewer intermediate processes. The coal carrier gas affects the hydrogen production only in the SCL system by altering the composition of syngas induced by gasifier temperature variation.

10/00085 Investigation of syngas ratio adjustment using a polyimide membrane

Peer, M. *et al. Chemical Engineering and Processing: Process Intensification*, 2009, 48, (3), 755–761.

In this work, separation of hydrogen from carbon monoxide by a polyimide hollow fibre membrane module was investigated. Polyimide showed high selectivity for hydrogen relative to carbon monoxide at different operational conditions. Effects of temperature, pressure and stage-cut on permeability of gases and membrane selectivity were experimentally studied. The experiments were carried out employing mixtures containing: 0, 10, 25, 40 and 50% carbon monoxide. Feed temperatures and pressures were varied between 20 and 80 °C and 5–9 bar, respectively. Pure gas permeances through the membrane were found to be nearly constant at different pressures. Also, the results confirmed the plasticization effect of carbon monoxide on the membrane and showed reduction of hydrogen permeance in mixed gas experiments due to competitive sorption and concentration polarization effects. Also, membrane area for a specific separation was calculated using a new developed model. The optimum condition which results in minimum required area for the membrane can be determined in this way.

10/00086 Reforming of methane over noble metal catalysts: catalyst deactivation induced by thiophene

Requies, J. *et al. Catalysis Today*, 2009, 143, (1–2), 9–16.
This work is focused on the performance of rhodium and ruthenium catalysts for the low temperature wet catalytic partial oxidation (LTCPO) of methane in sulfur-free conditions and also at different sulfur concentrations. Catalysts characterization was conducted by X-ray diffraction (XRD), BET surface area measurements, X-ray photoelectron spectroscopy (XPS), oxygen chemisorption by TGA, and transmission electron microscopy (TEM). All of the catalysts showed a high activity and selectivity towards hydrogen if sulfur-free reaction conditions were applied. The presence of small amounts of thiophene (10 ppm) in the feed decreased the activity for all the catalysts. However, at this concentration one ruthenium catalyst showed a high sulfur tolerance. For all the rhodium catalysts a strong deactivation and a higher carbon dioxide selectivity was observed at 10 ppm of thiophene. Operation with 400 ppm of thiophene in the feed resulted in a low activity for both Rh and Ru catalysts, and only a small amount of carbon dioxide was produced.

10/00087 Steady-state and transient hydrocarbon production in graphite by low energy impact of atomic and molecular deuterium projectiles

Zhang, H. and Meyer, F. W. *Journal of Nuclear Materials*, 2009, 390–391, 127–131.
This study reports measurements of steady-state yields of methyl, methane and heavier hydrocarbons for deuterium atomic and molecular ions incident on ATJ graphite, HOPG, and a-C:D thin films in the energy range 10–200 eV/D. The yields were determined using a QMS technique in conjunction with calibrated hydrocarbon leaks. The authors have also studied transient hydrocarbon production and hydrogen (deuterium) re-emission for 80 and 150 eV/D D^+, D_2^+, and D_3^+ projectiles incident on ATJ graphite surfaces pre-loaded to steady state by 20 eV/D beams of the corresponding species. Immediately after starting the higher-energy beams, transient hydrocarbon and D_2 re-emission yields significantly larger than steady-state values were observed, which exponentially decayed as a function of beam fluence. The initial yield values were related to the starting hydrocarbon and deuterium densities in the prepared sample, while the exponential decay constants provided information on the hydrocarbon kinetic release and hydrogen (deuterium) detrapping cross-sections.

10/00088 Study on a catalytic membrane reactor for hydrogen production from ethanol steam reforming

Yu, C.-Y. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 2947–2954.
Ethanol steam reforming in a membrane reactor with catalytic membranes was investigated to achieve important aims in one process, such as improvement in ethanol conversion and hydrogen yield, high hydrogen recovery and CO reduction. In order to confirm the efficiency of reaction and CO reduction, an ethanol reforming-catalytic membrane reactor with water–gas shift reaction (ECRW) in the permeate side was compared with a conventional reactor (CR) and an ethanol reforming-catalytic membrane reactor (ECR). In comparison with the CR, an ethanol conversion improvement of 11.9–19% and high hydrogen recovery of 78–87% were observed in the temperature range of 300–600 °C in the ECRW. Compared with CR and ECR, the hydrogen yield of ECRW increased up to 38% and 30%, respectively. Particularly, the ECRW showed higher hydrogen yield at high temperature, because Pt/Degussa P25 loaded in the permeate side showed catalytic activity for the methane steam reforming as well as WGS reaction. Moreover, CO concentration was reduced under 1% by the WGS reaction in the permeate side in the temperature range of 300–500 °C.

10/00089 Supercritical water gasification of Victorian brown coal: experimental characterisation

Yamaguchi, D. *et al. International Journal of Hydrogen Energy*, 2009, 34, (8), 3342–3350.
Supercritical water gasification is an innovative thermochemical conversion method for converting wet feedstocks into hydrogen-rich gaseous products. The non-catalytic gasification characteristics of Victorian brown coal were investigated in supercritical water by using a novel immersion technique with quartz batch reactors. Various operating parameters such as temperature, feed concentration and reaction time were varied to investigate their effect on the gasification behaviour. Gas yields, carbon gasification efficiency and the total gasification efficiency increased with increasing temperature and reaction time, and decreasing feed concentration. The mole fraction of hydrogen in the product gases was lowest at 600 °C, and increased to over 30% at a temperature of 800 °C. Varying parameters, especially reaction time, did not improve the coal utilization for gas production significantly and the measured data showed a large deviation from the equilibrium level.

LNG

10/00090 Analysis and optimization of a cascading power cycle with liquefied natural gas (LNG) cold energy recovery

Lu, T. and Wang, K. S. *Applied Thermal Engineering*, 2009, 29, (8–9), 1478–1484.
The effective utilization of the cryogenic energy associated with liquefied natural gas (LNG) vaporization is quite important. In this paper a cascading power cycle with LNG directly expanding consisting of a Rankine cycle with ammonia–water as working fluid and a power cycle of combustion gas is proposed to recover cryogenic energy of LNG. Energy equilibrium equations and exergy equilibrium equations of each equipment in the cascading power cycle are established. Taking some operating parameters as key parameters, influences of these parameters on thermal efficiency and exergy efficiency of the cascading power cycle were analysed. Optimization of the cascading power cycle with maximum economic benefits as objective function together with optimum variables and constraint conditions was solved. The optimum objective and variables were achieved.

10/00091 Nucleate pool boiling of liquid methane and its natural gas mixtures

Gong, M. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2733–2739.
An apparatus was designed and built for this study on pool-boiling heat transfer characteristics of pure and mixed fluids at cryogenic temperature. With this apparatus, extensive measurements were carried out to investigate the pool-boiling behaviours of pure methane and three binary mixtures of methane + ethane, methane + propane and methane + isobutane, as well as a multicomponent mixture of methane, ethane, propane and isobutane. The present measurements were performed in a descending heat flux procedure ranging from 250 kW/m^2 to 30 kW/m^2 at a fixed pressure of 0.13 MPa. Comprehensive measured data were presented in this paper, and also compared with some existing correlations. The deviations between the measured data and the predicted results locate within ±25% range.

10/00092 Queensland banks on coal-seam gas exports

Anon., *Oil and Energy Trends*, 2009, 34, (7), 7–8.
Australia's coal-bed methane industry has received a major boost from proposals by a number of companies to build terminals to export the gas as LNG. Seven consortia have submitted plans for terminals in Queensland, where the country's main reserves of coal-seam gas lie.

Hydrogen generation and storage

10/00093 Ammonia as a green fuel and hydrogen source for vehicular applications

Zamfirescu, C. and Dincer, I. *Fuel Processing Technology*, 2009, 90, (5), 729–737.
Ammonia, mostly known as a nitrogen feedstock for agriculture or as a refrigerant, has been occasionally used in the past as fuel for internal combustion engines and fuel cells. Because it is a carbon-free substance and has a high octane number there is currently a renewed interest for using ammonia as a fuel. The potential benefits and technical advantages of using ammonia as a sustainable fuel for power generation on vehicles are analysed here based on some performance indicators including the system effectiveness, the driving range, fuel tank compactness and the cost of driving. The cooling effect of ammonia is another advantage and is included in the efficiency calculations. Cooling with ammonia represents up to 20% from the engine's power, being a valuable side benefit of ammonia's presence on-board allowing for downsizing of the engine cooling system and obtaining some air conditioning. If the cooling effect is taken into consideration, the system's effectiveness can be improved by ~11%. It is shown that a medium-size hydrogen car converted to ammonia becomes more effective per driving range cost at CN$3.2/100 km and fuel tank compactness with 18 L/100 km with a cost of ammonia assumed to be CN$0.3/kg.

10/00094 Carbon dioxide capture with dolomite: a model for gas–solid reaction within the grains of a particulate sorbent

Stendardo, S. and Foscolo, P. U. *Chemical Engineering Science*, 2009, 64, (10), 2343–2352.

This work describes a mathematical model for a gas–solid reaction taking place within reactant particles made up of very small spherical grains, which grow during the reaction process due to solid product formation around the grain inner core, so that the particle void-fraction is reduced as the reaction proceeds. The structural changes in the spherical grains are taken into account in the proposed model by the inclusion of a variable diffusion coefficient of the gaseous reactant through the developing product layer. This progressively increasing transport resistance leads to a marked reduction in both reaction rate and sorbent capacity, as observed in practice in the carbonation of calcined dolomite, a process of importance in hydrogen production by means of coal or biomass gasification.

10/00095 Catalytic walls and micro-devices for generating hydrogen by low temperature steam reforming of ethanol

Casanovas, A. *et al. Catalysis Today*, 2009, 143, (1–2), 32–37.

Ethanol steam reforming ($S/C = 3$) was effectively performed at a low-temperature over catalytic wall reactors comprising a wide range of channel dimensions, ranging from conventional monoliths (channel width of 0.9 mm) to semicylindrical microchannels (0.35 mm radius) and to silicon micromonoliths (channel diameter of 3–4 μm). Co_3O_4 catalyst coatings were successfully prepared inside the channels from *in situ* thermal decomposition of two-dimensional layered cobalt hydroxide salts and showed a remarkable high homogeneity and mechanical stability. The Si-micromonolithic reactor proved extremely promising for hydrogen production for micro-fuel cell operation. Specific H_2 production rates exceeding 50 L_N of H_2 per mL of liquid and cm^3 of reactor were measured for c.42% ethanol conversion and residence times in the order of milliseconds.

10/00096 Easy synthesis of highly nitrogen-enriched graphitic carbon with a high hydrogen storage capacity at room temperature

Yang, S.-J. *et al. Carbon*, 2009, 47, (6), 1585–1591.

An easy method for synthesizing highly nitrogen-enriched graphitic carbon was developed and its hydrogen storage capacity was explored. The synthesis method uses a solution-based, stepwise condensation reaction between cyanuric chloride and melamine at low temperature (e.g. 0, 25, and 120 °C) and ambient pressure using conventional glassware without the need for an autoclave vessel. The physical and chemical structure of the synthesized highly nitrogen-enriched graphitic carbon was investigated by powder X-ray diffraction, scanning and transmission electron microscopy, selected area electron diffraction, energy dispersive spectroscopy, elemental analysis, Fourier transform infrared spectroscopy, X-ray photoemission spectroscopy, and electron energy loss spectroscopy. The analyses confirmed that the product has a highly crystalline nitrogen-enriched graphitic structure ($d_{002} = 0.324$ nm) with a carbon-to-nitrogen ratio of 1:1.12 (> 50 atomic% nitrogen content). The material was determined to have an excellent hydrogen storage capacity of 0.34 wt% at room temperature under 100 bar in spite of its low BET surface area of only 10 m^2/g.

10/00097 Effect of particle size on the electrochemical properties of $MmNi_{3.8}Co_{0.75}Mn_{0.4}Al_{0.2}$ hydrogen storage alloy

Zhao, X. *et al. International Journal of Hydrogen Energy*, 2009, 34, (8), 3389–3394.

Charge and discharge testing, linear polarization, electrochemical impedance spectroscopy (EIS) and potential step chronoamperometry (PSCA) were used to investigate the electrochemical properties of the Ce-rich mischmetal $MmNi_{3.8}Co_{0.75}Mn_{0.4}Al_{0.2}$ hydrogen storage alloy with different particle sizes. At a discharge current density of 900 mA/g, the alloy with small original particle size maintained a high rate dischargeability (HRD) above 86% while the alloy with large particle size could not discharge in the same potential region. The alloy with small original particle size also showed lower contact resistances and polarization resistance after full activation. Both the exchange current density and the hydrogen diffusion coefficient increased when the hydrogen concentration decreased. The charge-transfer reaction on the surface of alloy particles with different sizes should be mainly responsible for the differences in electrochemical properties, especially the HRD.

10/00098 Effect of substituting Al for Co on the hydrogen-storage performance of $La_{0.7}Mg_{0.3}Ni_{2.6}Al_xCo_{0.5-x}$ ($x = 0.0$–0.3) alloys

Liu, Y. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 2986–2991.

$La_{0.7}Mg_{0.3}Ni_{2.6}Al_xCo_{0.5-x}$ ($x = 0.0$–0.3) alloys were prepared by induction melting, and the effects of partially substituting Al for Co on the structure and hydrogen-storage properties of the alloys were investigated systematically. It is found that La(Ni, Co, Al) $_5$ phase with hexagonal $CaCu_5$-type structure, $LaNi_3$ phase with $PuNi_3$ structure and $MgNi_2$ phase exist as the main phases in $La_{0.7}Mg_{0.3}Ni_{2.6}Al_xCo_{0.5-x}$ ($x = 0.0$–0.3) alloys, and the cell volume of the La(Ni, Co, Al)$_5$ phase increases with the amount of Al added. The results show that the substitution of Al for Co can reduce the plateau pressure and the hysteresis between hydrogen absorption and desorption, and improve the hydrogen-absorption capacity and thermal stability of the hydride. Moreover, the addition of Al can delay the oxidation of the surface layer of the alloy electrodes in electrolyte, slow down the capacity degradation and prolong the cycling lifetime, and enhance the electrocatalytic activity of the hydrogen-storage electrodes for hydrogen oxidation.

10/00099 Gas and particle circulation in an internally circulating fluidized bed membrane reactor cold model

Xie, D. *et al. Chemical Engineering Science*, 2009, 64, (11), 2599–2606.

A cold model study was carried out of an internally circulating fluidized bed membrane reactor for hydrogen production by steam reforming. This configuration facilitates a novel process in which air is introduced for autothermal operation, while avoiding diluting the hydrogen in the gas stream by nitrogen. A column of diameter 230 mm and height 2.4 m contained a membrane box of square cross-section. Gas circulation was investigated by injecting helium tracer into the top of the bed above the membrane box and detecting its concentration in the annulus and lower membrane box by a thermal conductivity detector. Solids circulation was determined from the downward velocity of particles in the annulus. The major resistance to solids circulation was found to be at the passage connecting the outer downflow to the inner upflow compartment. A ring distributor helped overcome this resistance.

10/00100 High capacity hydrogen storage in a hybrid ammonia borane–lithium amide material

Graham, K. R. *et al. Energy Environmental Science*, 2009, 2, (7), 706–710.

The direct (solventless) reaction of lithium amide with ammonia borane is described and is demonstrated to form a new hybrid material approximating to $LiNH_2BH_3NH_3$. This material rapidly loses 3.2 mole equivalents of hydrogen, (11.9 wt%) on heating to 250 °C, with the most rapid hydrogen release occurring at temperatures as low as 60 °C. The product was an insoluble, amorphous polymer with the general formula $-(NLi-BNH_2)_n-$ which did not rehydrogenate directly on exposure to hydrogen gas pressure. The hybrid material and its decomposition products were characterized by solid state ^{11}B NMR. Selective deuterium labelling helped to elucidate a reaction sequence for the hydrogen release using mass spectrometry of the released gases.

10/00101 High yield conversion of a crude glycerol fraction from biodiesel production to hydrogen by photofermentation

Sabourin-Provost, G. and Hallenbeck, P. C. *Bioresource Technology*, 2009, 100, (14), 3513–3517.

Present biodiesel manufacturing processes inevitably produce a crude glycerol side fraction. Projected future volumes of biodiesel will generate enormous quantities of glycerol of a magnitude suggesting that conversion to a fuel is the only viable route. Here it was shown that the photosynthetic bacterium *Rhodopseudomonas palustris* is capable of the photofermentative conversion of glycerol, both pure and a crude glycerol fraction, to hydrogen, a proposed future fuel. Relatively high yields, up to 6 moles H_2/mole glycerol (75% of theoretical, 8 moles of H_2/mole glycerol) were obtained. Even the crude glycerol fraction, at the concentrations used here, was readily converted to hydrogen with no apparent evidence of inhibition or toxicity. It is shown that the concentration of added nitrogen can be used to modify both rates and yields of hydrogen production with an apparent trade-off between the two. Finally, some factors are identified that might be examined in future studies in attempts to increase rates and/or yields.

10/00102 Hollow Ni–SiO_2 nanosphere-catalyzed hydrolytic dehydrogenation of ammonia borane for chemical hydrogen storage

Umegaki, T. *et al. Journal of Power Sources*, 2009, 191, (2), 209–216.

Nickel clusters contained within silica nanospheres (20–30 nm) were synthesized by using a $Ni(NH_3)_6Cl_2$ crystal template method in a polyoxyethylene–nonylphenyl ether/cyclohexane reversed micelle system followed by an *in situ* reduction in aqueous $NaBH_4/NH_3BH_3$ solutions. Metallic nickel clusters exist inside the SiO_2 nanospheres prepared by the method while oxidized nickel clusters prepared by the conventional impregnation method were supported on the outer surface of silica as shown in the results of transmission electron microscope/energy dispersive X-ray and X-ray photoelectron spectroscopy measurements. The nickel clusters inside of silica nanospheres show higher catalytic activity for hydrolysis of ammonia borane to generate stoichiometric amount of hydrogen than the supported nickel catalysts.

10/00103 Hydrogen from alcohols: IR and flow reactor studies

Busca, G. *et al. Catalysis Today*, 2009, 143, (1–2), 2–8.

The reactions of methanol and ethanol steam reforming (MSR and ESR) have been studied over Cu–ZnO–Al_2O_3 and over Ni-containing catalysts, respectively. These spectroscopic studies, coupled with flow reactor studies, allowed the proposed mechanisms for both reactions where water takes the role of oxidant of part of the copper and nickel species. The incompletely reduced catalysts convert the alcohols into formate and acetate species, respectively, plus gas phase hydrogen. Over Cu–ZnO–Al_2O_3 formates decompose into adsorbed CO which is rapidly oxidized into CO_2 before leaving the surface. This allows CO production lower than forecast from the water gas shift (WGS) equilibrium. Over Ni-based catalysts acetates decompose into CO and methane. In fact, the ESR reaction was found to produce, above 700 K, hydrogen, carbon oxides and methane. The formation of hydrogen is limited by the establishing of the WGS (which would likely unavoidably limit the one-step production of hydrogen by ESR) and the methane SR equilibria. Activation of the C2 carbon atom of ethanol or of some of its decomposition products would be needed to avoid methane formation, thus increasing hydrogen yield. Preliminary work on isopropanol SR was performed over a Pd–Cu catalyst. Cracking and production of methane lower significantly the selectivity to CO_x and hydrogen.

10/00104 Hydrogen production by sorption-enhanced steam reforming of glycerol

Dou, B. *et al. Bioresource Technology*, 2009, 100, (14), 3540–3547.

Catalytic steam reforming of glycerol for H_2 production has been evaluated experimentally in a continuous flow fixed-bed reactor. The experiments were carried out under atmospheric pressure within a temperature range of 400–700 °C. A commercial Ni-based catalyst and a dolomite sorbent were used for the steam reforming reactions and *in situ* CO_2 removal. The product gases were measured by on-line gas analysers. The results show that H_2 productivity is greatly increased with increasing temperature and the formation of methane by-product becomes negligible above 500 °C. The results suggest an optimal temperature of 500 °C for the glycerol steam reforming with *in situ* CO_2 removal using calcined dolomite as the sorbent, at which the CO_2 breakthrough time is longest and the H_2 purity is highest. The shrinking core model and the one-dimensional diffusion model describe well the CO_2 removal under the conditions of this work.

10/00105 Hydrogen storage properties of Mg–Ni–Cu prepared by hydriding combustion synthesis and mechanical milling (HCS + MM)

Gu, H. *et al. International Journal of Hydrogen Energy*, 2009, 34, (6), 2654–2660.

The effect of Cu-doping on the hydrogen storage properties of $Mg_{95}Ni_5Cu_x$ ($x = 0$, 0.5, 1, 2) prepared by hydriding combustion synthesis and mechanical milling (HCS + MM) was studied. For dehydriding properties, the dehydriding temperature onset decreases from 450 K for $Mg_{95}Ni_5$ to 420 K for $Mg_{95}Ni_5Cu_2$. Additionally, the activation energy for dehydriding decreases from 116 kJ/mol for $Mg_{95}Ni_5$ to 98 kJ/mol for $Mg_{95}Ni_5Cu_2$, indicating that the dehydriding reaction is activated by the catalytic effect of Cu. Moreover, the hydrogen absorption capacity of $Mg_{95}Ni_5Cu_2$ at 373 K in 100 s increases from 0.95 to 4.16 wt% by MM pretreatment before HCS. The factors for the improvement of the hydrogen storage properties are discussed in this paper.

10/00106 Improved synthesis and hydrogen storage of a microporous metal–organic framework material

Cheng, S. *et al. Energy Conversion and Management*, 2009, 50, (5), 1314–1317.

A microporous metal–organic framework MOF-5 [$Zn_4O(BDC)_3$, BDC = 1,4-benzenedicarboxylic] was synthesized with and without H_2O_2 by improved methods based on the previous studies. The obtained materials were characterized by X-ray diffraction, scanning electron microscopy and nitrogen adsorption, and their hydrogen storage capacities were measured. The synthesis experiments showed that H_2O_2 favoured the growth of high quality sample, large pore volume and high specific surface area. The measurements of hydrogen storage indicated that the sample with higher specific surface area and large pore volume showed better hydrogen storage behaviour than other samples. It was suggested that specific surface area and pore volume influenced the capacity of hydrogen storage for MOF-5 material.

10/00107 Improving hydrogen storage in Ni-doped carbon nanospheres

Zubizarreta, L. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 3070–3076.

The effect of nickel distribution and content in Ni-doped carbon nanospheres on hydrogen storage capacity under conditions of moderate temperature and pressure was studied. It was found that the nickel distribution, obtained by using different doping techniques and conditions, has a noticeable influence on hydrogen storage capacity. The samples with the most homogeneous nickel distribution, obtained by pre-oxidizing the carbon nanospheres, displayed the highest storage capacity. In addition, storage capacity is influenced by the amount of nickel. It was found a higher storage capacity in samples containing 5 wt% of Ni. This is due to the greater interactions between the nickel and the support that produce a higher activation of the solid through a spillover effect.

10/00108 Kinetic models for fermentative hydrogen production: a review

Wang, J. and Wan, W. *International Journal of Hydrogen Energy*, 2009, 34, (8), 3313–3323.

The kinetic models were developed and applied for fermentative hydrogen production. They were used to describe the progress of a batch fermentative hydrogen production process, to investigate the effects of substrate concentration, inhibitor concentration, temperatures, pH, and dilution rates on the process of fermentative hydrogen production, and to establish the relationship among the substrate degradation rate, the hydrogen-producing bacteria growth rate and the product formation rate. This review showed that the modified Gompertz model was widely used to describe the progress of a batch fermentative hydrogen production process, while the Monod model was widely used to describe the effects of substrate concentration on the rates of substrate degradation, hydrogen-producing bacteria growth and hydrogen production. Arrhenius model was used a lot to describe the effects of temperature on fermentative hydrogen production, while modified Han–Levenspiel model was used to describe the effects of inhibitor concentration on fermentative hydrogen production. The Andrew model was used to describe the effects of H^+ concentration on the specific hydrogen production rate, while the Luedeking–Piret model and its modified form were widely used to describe the relationship between the hydrogen-producing bacteria growth rate and the product formation rate. Finally, some suggestions for future work with these kinetic models were proposed.

10/00109 Manipulating the hydrogen production from acetate in a microbial electrolysis cell–microbial fuel cell-coupled system

Sun, M. *et al. Journal of Power Sources*, 2009, 191, (2), 338–343.

A biological hydrogen-producing system is configured through coupling an electricity-assisting microbial fuel cell (MFC) with a hydrogen-producing microbial electrolysis cell (MEC). The advantage of this biocatalysed system is the *in situ* utilization of the electric energy generated by an MFC for hydrogen production in an MEC without external power supply. In this study, it is demonstrated that the hydrogen production in such an MEC–MFC-coupled system can be manipulated through adjusting the power input on the MEC. The power input of the MEC is regulated by applying different loading resistors connected into the circuit in series. When the loading resistance changes from 10 Ω to 10 kΩ, the circuit current and volumetric hydrogen production rate varies in a range of 78 ± 12 to $9 \pm 0\,\mathrm{mA\,m^{-2}}$ and 2.9 ± 0.2 to $0.2 \pm 0.0\,\mathrm{mL\,L^{-1}\,d^{-1}}$, respectively. The hydrogen recovery (R_{H_2}), Coulombic efficiency, and hydrogen yield (Y_{H_2}) decrease with the increase in loading resistance. Thereafter, in order to add power supply for hydrogen production in the MEC, additional one or two MFCs are introduced into this coupled system. When the MFCs are connected in series, the hydrogen production is significantly enhanced. In comparison, the parallel connection slightly reduces the hydrogen production. Connecting several MFCs in series is able to effectively increase power supply for hydrogen production, and has a potential to be used as a strategy to enhance hydrogen production in the MEC–MFC-coupled system from wastes.

10/00110 Nuclear heat for hydrogen production: coupling a very high/high temperature reactor to a hydrogen production plant

Elder, R. and Allen, R. *Progress in Nuclear Energy*, 2009, 51, (3), 500–525.

Hydrogen produced from water splitting, as opposed to from hydrocarbons, has the potential to be a carbon neutral energy solution. There are several methods to extract hydrogen from water, three leading candidates being high temperature electrolysis, the SI thermochemical cycle and the HyS hybrid thermochemical cycle. All three of these processes involve a section requiring very high temperatures. The very high temperature reactor (VHTR), a gas cooled Generation IV reactor, is ideally suited for providing this high temperature heat. Nuclear hydrogen production is being investigated around the world. The four leading consortiums are the Japan Atomic Energy Agency (JAEA), PBMR/Westinghouse, GA, and AREVA NP/CEA/EDF. There are also many smaller R&D efforts focussing on the development of particular materials and components and on process flowsheeting. A nuclear hydrogen plant involves four key pieces of equipment: the VHTR, the hydrogen production plant (HPP), the intermediate heat exchanger (IHX) and the power conversion system (PCS). The choice of all four items varies dramatically between programmes. Both pebble bed and prismatic fuel block VHTRs are being developed, which can be directly or indirectly coupled to a HPP and PCS placed either in series or parallel. Either a Rankine steam cycle or a Brayton gas turbine cycle can be employed in the PCS. This report details the choices made and research being carried out around the world. Predicted process efficiencies and plant costs are currently at a preliminary stage and are very similar, regardless of the options chosen. The cost of hydrogen produced from water splitting using nuclear technologies is around \$2/kg H_2. This is competitive with hydrogen produced by other methods, particularly if carbon emissions are regulated and costed. The technological feasibility and testing of key components will be one of the determining factors in plant viability.

10/00111 Optimized heat transfer fin design for a metal-hydride hydrogen storage container

Melnichuk, M. *et al. International Journal of Hydrogen Energy*, 2009, 34, (8), 3417–3424.

This paper presents a heat transfer fin optimization for a $LaNi_5$ hydrogen storage container. In this simplified approach, a one-dimension fin model is proposed in order to avoid geometrical restrictions and constrains associated to a particular technological solution. Therefore, the presented model can be utilized as a general framework for the development of containers with inner fins. The hydrogen absorption reaction was simulated using a developed finite difference method. On this base, the heat transfer fin design was optimized for different absorption times and container diameters applying the gradient method. Numerical outcomes were then confirmed by comparison with experimental measurements, showing good agreement between the theoretical model and the experimental result.

10/00112 Sodium borohydride *versus* ammonia borane, in hydrogen storage and direct fuel cell applications

Demirci, U. B. and Miele, P. *Energy Environmental Science*, 2009, 2, (6), 627–637.

Since the late 1990s, sodium borohydride ($NaBH_4$, denoted SB) is presented as a promising hydrogen storage material and an attractive fuel (aqueous solution) of the direct fuel cell (or direct liquid-feed fuel cell). In 2007, the US Department of Energy recommended a no-go for SB for vehicular applications and suggested work on ammonia borane (AB), another promising hydrogen storage material, which is also considered as a fuel for the direct fuel cell. Both boron hydrides in hydrogen and fuel cell applications are the topics of the present paper. The basics, issues, solutions to the issues and state-of-the-art are tackled but the discussion aims to compare the hydrides for either application. It is shown that there are many similarities between SB and AB in their features and applications. Nevertheless SB and AB as hydrogen storage materials do not compete. Rather, SB is intended more to portable technologies while AB to vehicular applications. Otherwise, when these hydrides are utilized as fuels of direct fuel cell, one question arises: what can be the advantage of developing the AB-powered fuel cell when it seems to be less effective, practical, and more complex than the SB-powered fuel cell? These aspects are discussed. However that may be, it is concluded that both SB and AB are not mature enough for the applications considered.

10/00113 Ternary cobalt spinel oxides for solar driven hydrogen production: Theory and experiment

Walsh, A. *et al. Energy Environmental Science*, 2009, 2, (7), 774–782.

Discovery of a chemically stable, light absorbing and low resistivity metal oxide with band edges aligned to the water redox potentials has been a goal of physical scientists for the past forty years. Despite an immense amount of effort, no solution has been uncovered. We present a combined theoretical and experimental exploration of a series of unconventional ternary cobalt spinel oxides, which offer chemical functionality through substitution on the octahedral spinel B site. First-principles predictions of the substitution of group 13 cations (Al, Ga, In) in Co_3O_4 to form a series of homologous CoX_2O_4 spinel compounds are combined with experimental synthesis and photoelectrochemical characterization. Ultimately, while tunable band gaps in the visible range can be obtained, the material performance is limited by poor carrier transport properties associated with small polaron carriers. Future design pathways for metal oxide exploration are discussed.

10/00114 The steam reforming of phenol over natural calcite materials

Constantinou, D. A. and Efstathiou, A. M. *Catalysis Today*, 2009, 143, (1–2), 17–24.

Five natural calcite materials of different geographical origin were studied in the steam reforming of phenol and the activity results obtained were correlated with some of their physico-chemical properties. It was found that the specific catalytic activity $(\mu mol/(m^2 s))$ of the calcite material following calcination at 850 °C was not correlated with the BET area and the primary crystal size of calcium oxide (CaO). The metal impurity levels of the natural calcite materials investigated were found to be very low as evidenced by EDX and XPS measurements, leading to the conclusion that their effect on the catalytic chemistry of phenol steam reforming and surface adsorption properties of CaO was minor. These results suggest that the reaction depends on the heterogeneity and site reactivity present in each CaO surface examined. On the other hand, based on diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) CO_2 chemisorption and TPD-CO_2 mass spectrometry studies, it was found that the catalytic activity can be correlated with the amount of CO_2 adsorbed at 25 °C in the unidentate form. The latter species was found to be significantly more thermally stable than the bicarbonate adsorbed species also populated on the CaO surface after CO_2 chemisorption (15 Torr) at 25 °C. The least concentration of unidentate carbonate species accumulated on the catalyst surface the higher the catalytic activity of CaO to be expected. It was found that the presence of hydrogen in the feed stream results in a significant decrease of steam reforming of phenol activity over CaO. This result was probed to be likely related to the reduction in the rate of water dissociation to form –OH species, as revealed by the significant decrease in the concentration of adsorbed bicarbonate and –OH species on the surface of CaO according to *in situ* DRIFTS-CO_2 adsorption experiments in the presence of water and of varying hydrogen concentration in the feed. The inhibiting role of H_2 during steam reforming of phenol over CaO is discussed.

10/00115 Thermodynamic analysis of two-step solar water splitting with mixed iron oxides

Roeb, M. *et al. International Journal of Energy Research*, 2009, 33, (10), 893–902.

A two-step thermochemical cycle for solar production of hydrogen from water has been developed and investigated. It is based on metal oxide redox pair systems, which can split water molecules by abstracting oxygen atoms and reversibly incorporating them into their lattice. After successful experimental demonstration of several cycles of alternating hydrogen and oxygen production, the present work describes a thermodynamic study aiming at the improvement of process conditions and at the evaluation of the theoretical potential of the process. In order to evaluate the maximum hydrogen production potential of a coating material, theoretical considerations based on thermodynamic laws and properties are useful and faster than actual tests. Through thermodynamic calculations it is possible to predict the theoretical maximum output of H_2 from a specific redox-material under certain conditions. Calculations were focused on the two mixed iron oxides nickel-iron-oxide and zinc-iron-oxide. In the simulation the amount of oxygen in the redox-material is calculated before and after the water-splitting step on the basis of laws of thermodynamics and available material properties for the chosen mixed iron oxides. For the simulation the commercial Software FactSage and available databases for the required material properties were used. The analysis showed that a maximum hydrogen yield is achieved if the reduction temperature is raised to the limits of the operation range, if the temperature for the water splitting is lowered below 800°C and if the partial pressure of oxygen during reduction is decreased to the lower limits of the operational range. The predicted effects of reduction temperature and partial pressure of oxygen could be confirmed in experimental studies. The increased hydrogen yield at lower splitting temperatures of about 800°C could not be confirmed in experimental results, where a higher splitting temperature led to a higher hydrogen yield. As a consequence it can be stated that kinetics must play an important role especially in the splitting step.

10/00116 Viable storage of hydrogen in materials with off-board recharging using high-temperature electrolysis

Løvvik, O. M. *International Journal of Hydrogen Energy*, 2009, 34, (6), 2679–2683.

Hydrogen storage in materials (hydrides) is challenging for vehicular applications, due to the large amounts of heat that must be removed in a short period of time during the filling process. It is proposed that rehydrogenation of the hydride instead is performed outside the vehicle, and linked to hydrogen production by water electrolysis at the filling station. The waste heat removed from the hydride during filling can be used to heat the electrolysis cell, increasing its efficiency. This solution can speedup the filling process, increase the efficiency of the hydrogen production, increase safety during filling, eliminate the need for massive transportation of hydrogen, and open the arena for many new hydrogen storage materials.

04 BY-PRODUCTS RELATED TO FUELS

10/00117 Adsorption of carbon dioxide using impregnated activated carbon promoted by Zinc

Somy, A. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (3), 249–254.

The effect of impregnation of activated carbon with Cr_2O and Fe_2O_3 and promotion by Zn^{2+} on its adsorptive properties of carbon dioxide was studied using a volumetric adsorption apparatus at ambient temperature and low pressures. Slurry and solution impregnation methods were used to compare CO_2 capture capacity of the impregnated activated carbon promoted by Zinc. The obtained adsorption isotherms showed that amount of CO_2 adsorbed on the samples impregnated by Cr_2O was increased about 20% in compare to raw activated carbon. The results also showed that Fe_2O_3 was not an effective impregnating species for activated carbon modification. Moreover slurry impregnation method showed higher CO_2 adsorption capacity in comparison with solution impregnation method. Samples prepared by co-impregnation of two metal species showed more adsorption capacity than samples impregnated by just one metal species individually. Washing the impregnated samples by metal oxide resulted in 15% increase in CO_2 adsorption capacities of activated carbons which can be attributed to the metal oxides removal covering the adsorption surface. Decreasing impregnation temperature from 95 to 25 °C in solution method showed a significant increase in CO_2 adsorption capacity. Sips equation was found a suitable model fitting to the adsorption data in the range studied.

10/00118 Chemical fractionation for the characterisation of fly ashes from co-combustion of biofuels using different methods for alkali reduction

Pettersson, A. *et al. Fuel*, 2009, 88, (9), 1758–1772.

Chemical fractionation, SEM–EDX and XRD was used for characterization of fly ashes from different co-combustion tests in a 12 MW circulating fluidized bed boiler. The fuels combusted were wood pellets as base fuel and straw pellets as co-fuel in order to reach a fuel blend with high alkali and chlorine concentrations. This fuel blend causes severe problems with both agglomeration of bed material if silica sand is used and with deposits in the convection section of the boiler. Counter measures to handle this situation and avoiding expensive shut downs, tests with alternative bed materials and additives were performed. Three different bed materials were used; silica sand, Olivine sand and blast furnace slag (BFS) and different additives were introduced to the furnace of the boiler; kaolin, zeolites and sulfur with silica sand as bed material. The results of the study are that BFS gives the lowest alkali load in the convection pass compared with silica and olivine sand. In addition less alkali and chlorine was found in the fly ashes in the BFS case. The Olivine sand however gave a higher alkali load in the convection section and the chemical fractionation showed that the main part of the alkali in the fly ashes was soluble, thus found as KCl which was confirmed by the SEM–EDX and XRD. The comparison of the different additives gave that addition of Kaolin and Zeolites containing aluminium-silicates captured 80% of the alkali in the fly ash as insoluble alkali–aluminium-silicates and reduced the KCl load on the convection section. Addition of sulfur reduced the KCl load in the flue gas even more but the K_2SO_4 concentration was increased and KCl was found in the fly ashes anyhow. The chemical fractionation showed that 65% of the alkali in the fly ashes of the sulfur case was soluble.

10/00119 Hydrogen storage evaluation based on investigations of the catalytic properties of metal/metal oxides in electrospun carbon fibers

Im, J. S. *et al. International Journal of Hydrogen Energy*, 2009, 34, (8), 3382–3388.

In order to investigate the catalytic capacity of metals and metal oxides based on electrospun carbon fibres for improving hydrogen storage, electrospinning and heat treatments were carried out to obtain metal/metal oxide-embedded carbon fibres. Although the fibres were treated with the same activation procedure, they had different pore structures, due to the nature of the metal oxide. When comparing the catalytic capacity of metal and metal oxide, metal exhibits better performance as a catalyst for the improvement of hydrogen storage, when considering the hydrogen storage system. When a metal oxide with an m.p. lower than the temperature of heat treatment was used, the metal oxide was changed to metal during the heat treatment, developing a micropore structure. The activation process produced a high specific surface area of up to 2900 m^2/g and a pore volume of up to 2.5 cm^3/g. The amount of hydrogen adsorption reached approximately 3 wt% at 100 bar and room temperature.

10/00120 Investigation on thermal radiation spectra of coal ash deposits

Saljnikov, A. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2871–2884.

This paper deals with thermal radiation properties of ash deposits on a pulverized coal boiler of an electric power plant. Normal emittance spectra in the 2.5–25 μm interval, and total normal emittance, were measured on four kinds of ash layers of a mm magnitude order thickness, at $560 \rightarrow 1460 \rightarrow 560$ K in heating and cooling. It was found that ash powder layers are opaque for infrared radiation. The emittance increases with ash radiation wavelength and temperature. Ash powder is sintered and fused above 1200 K. The emittance of the sintered layer is above that of the unsintered layer. The authors propose, and explain by an example, correlating the experimentally obtained emittance spectra of ash deposits with a continuous curve, the formula of which defines the dependence of emittance on wavelength and temperature, i.e. $\epsilon = \epsilon(\lambda,\tau)$. Use of this formula, with parameter values determined by the proposed methodology, may greatly simplify the practical application of the experimentally determined emittances in the thermal design of existing and new steam boiler furnaces.

10/00121 Microstructure changes and properties of TiC-coated carbon fiber-reinforced carbon composites

Wang, K. *et al. Fusion Engineering and Design*, 2009, 83, (4), 644–648.

In the present paper, X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) were used to study distortion of TiC crystals after thermal cycles in plasma environment. Scanning electron microscopy (SEM) was used to observe morphology changes and penetrating cracks in TiC/C coatings. To avoid the cracks and enhance properties of coated carbon fibre-reinforced carbon (C/C) composites, TiC/C composites were prepared as buffer layer to relieve thermal stresses. Thermal cycles indicated that the buffer layer could effectively improve thermal shock resistance of pure TiC coated C/C composites. To study the reason, transmission electron microscopy (TEM) results suggested that TiC particles were uniformly imbedded in pyrocarbon in the buffer layer, which was advantageous to relieve mismatch of coefficient of thermal expansion (CTE) between pure TiC and C/C. Moreover, thermal conductivity tests showed that the buffer layer was in favour of transferring heat loading.

10/00122 Production of hydrogen and syngas via gasification of the corn and wheat dry distiller grains (DDGS) in a fixed-bed micro reactor

Tavasoli, A. *et al. Fuel Processing Technology*, 2009, 90, (4), 472–482.

Production of hydrogen and syngas via gasification of the corn and wheat dry distiller grains (DDGS) with oxygen in a continuous downflow fixed bed micro reactor are studied in this paper. A series of experiments have been performed to investigate the effects of reaction time (15–45 min), reactor temperature (700–900 °C) and oxygen to nitrogen ratio (0.08–0.2 vol./vol.) on product gas composition, gas yield, low heating value (LHV) and carbon conversion efficiency. Over the ranges of the experimental conditions used, the results obtained seemed to suggest that for both biomasses the operating conditions were optimized for a gasification temperature around 900 °C, an oxygen to nitrogen ratio of 0.08 and a reaction time of 30 min, because a gas richer in hydrogen and carbon monoxide and poorer in carbon dioxide and hydrocarbons. The results showed that the product gas of corn DDGS gasification has higher H_2 and CO concentrations (11 and 56.5%) than that of wheat DDGS gasification (10.5 and 51.5%). In addition gasification of corn DDGS resulted to higher gas yield (0.42 m^3/kg), LHV (10.65 MJ/m^3) and carbon conversion efficiency (44.2%).

10/00123 The syngas production by partial oxidation using a homogeneous charge compression ignition engine

Yang, Y. C. *et al. Fuel Processing Technology*, 2009, 90, (4), 553–557.

This research studies the production of syngas from methane or simulated biogas with a HCCI reforming engine. Experiments were conducted on the changes in syngas concentration according to the variations of oxygen/methane ratio, total flow rate, intake heating temperature, CO_2 in mixture and oxygen enrichment with partial oxidation. Through the parametric screening studies, optimum conditions and their results in this study were obtained. The maximum content of syngas was; 27.4% at 0.3 of oxygen/methane ratio, 32.38% at 117.3 L/min of total flow rate, and 35.83% at 355 °C of intake heating temperature. A total of 41.06% of syngas was produced at 50.33% of oxygen enrichment ratio.

05 NUCLEAR FUELS

Scientific, technical

10/00124 2D divertor design calculations for the national high-power advanced torus experiment

Canik, J. M. *et al. Journal of Nuclear Materials*, 2009, 390–391, 315–318.

The national high-power advanced torus experiment is a concept for a new facility to address the FESAC theme of 'taming the plasma-material interface'. This concept exploits the compactness and excellent access provided by low aspect ratio to achieve a high ratio of exhaust power to major radius in order to study the integration of high-performance, long-pulse plasmas with a reactor-relevant high heat flux plasma boundary. Predictions of the scrape-off-layer plasma characteristics are presented, as calculated with the 2D edge modelling code SOLPS. Calculations in a variety of magnetic geometries indicate that very high levels of divertor heat flux can be expected, with peak values far in excess of the power handling capabilities of presently used materials. Possible methods to reduce the heat flux to acceptable levels are discussed.

10/00125 A thermal-hydraulic code (THYD) for the miniature neutron source reactor thermal-hydraulic transients

Albarhoum, M. and Mohammed, S. *Progress in Nuclear Energy*, 2009, 51, (3), 470–473.

The transient thermal-hydraulic problem of MNSR is represented by ten differential equations solved numerically using Runge–Kutta method. Computational results are then compared with experimental measurements. Fuel grids and cooling coil models are incorporated in the model too. Radiating energy from the clad is taken into account in the energy balance in the reactor. The pool is divided into three sections in the model. The effect of the cooling coil of the pool upper section on reactor thermal-hydraulic parameters is discussed. The only input parameter of the reactor is the power temporal distribution. Good agreement between calculated and measured data was obtained.

10/00126 Adsorption capacity of hydrogen isotopes on mordenite

Kawamura, Y. *et al. Fusion Engineering and Design*, 2009, 83, (4), 655–660.

In a fusion reactor system, a monitoring of hydrogen isotopes including tritium is necessary for the safety of system control and operation. A gas chromatography using a cryogenic separation column is one of the methods for hydrogen isotope analysis. Synthesis zeolite such as molecular sieve 5A (CaA) is a candidate material of the separation column, and its property varies by the ratio of silica to alumina, the kinds of cation and so on. If the factor affected the hydrogen adsorption property of the synthesis zeolite is clarified, it may lead to the development of the new zeolite optimized to the separation column. So, in this work, adsorption capacity of hydrogen (H_2) and deuterium (D_2) for mordenite (MOR) and NaY type zeolite (NaY) were investigated at various temperatures, and were compared with CaA. The amount of adsorption per unit weight of MOR was larger than that of CaA, and that of NaY was smaller than that of CaA. The adsorption isotherms were expressed by sum of two Langmuir equations, and the Langmuir coefficients of H_2 and D_2 were proposed. Furthermore, the Langmuir coefficients of HD, HT, DT and T_2 were estimated by the reduced mass. The correlation between the adsorption properties and the physical parameters of the zeolite were not confirmed.

10/00127 Analysis of low Reynolds number turbulent flow phenomena in nuclear fuel pin subassemblies of tight lattice configuration

Ninokata, H. *et al. Nuclear Engineering and Design*, 2009, 239, (5), 855–866.

This paper focuses on the numerical simulation of low Reynolds (Re) number turbulence flow phenomena in tightly packed fuel pin subassemblies and in channels of irregular shape such as eccentric annuli. Highlighted phenomena include (i) turbulence-driven secondary flows inside a subchannel, (ii) local turbulent-laminar transition in the narrow gap region, and (iii) global flow pulsation across the gap along the channel length. These phenomena are simulated by Computational Fluid Dynamics (CFD). The CFD methods employed here are those of Direct Numerical Simulation (DNS) of turbulence, Large Eddy Simulation (LES) and Reynolds-Averaged Navier–Stokes (RANS) equations approach. Complicated turbulent flow structure is due to strong anisotropy in the non-uniform channel geometry that is characterized by wide open channels connected by a narrow gap. The secondary flows in subchannels play an important role in transporting small eddies generated in the wider region toward the narrow gap. Periodic cross-flow oscillations are calculated to appear in the vicinity of the gap region, and the coherent structure is transported in the main flow direction. This macroscopic flow process prevails in the low Re turbulent flow regime and is called as global flow pulsation. Finally a brief discussion is made on their influences onto the mixing between two subchannels that must be taken into account during natural circulation decay heat removals.

10/00128 Burn up calculations for the Iranian miniature reactor: a reliable and safe research reactor

Faghihi, F. and Mirvakili, S. M. *Nuclear Engineering and Design*, 2009, 239, (6), 1000–1009.

Presenting neutronic calculations pertaining to the Iranian miniature research reactor is the main goal of this article. This is a key to maintaining safe and reliable core operation. The following reactor core neutronic parameters were calculated: clean cold core excess reactivity (ρex), control rod and shim worth, shut down margin (SDM), neutron flux distribution of the reactor core components, and reactivity feedback coefficients. Calculations for the fuel burnup and radionuclide inventory of the Iranian miniature neutron source reactor (MNSR), after 13 years of operational time, are carried out. Moreover, the amount of uranium burnup and produced plutonium, the concentrations and activities of the most important fission products, the actinide radionuclides accumulated, and the total radioactivity of the core are estimated. Flux distribution for both water and fuel temperature increases are calculated and changes of the central control rod position are investigated as well. Standard neutronic simulation codes WIMS-D4 and CITATION are employed for these studies. The input model was validated by the experimental data according to the final safety analysis report (FSAR) of the reactor. The total activity of the MNSR core is calculated including all radionuclides at the end of the core life and it is found to be equal to $1.3 \times 10^3 Ci$. This investigation shows that the reactor is operating under safe and reliable conditions.

10/00129 Burnable poison for reactivity management in a very high temperature reactor

Jo, C. K. *et al. Annals of Nuclear Energy*, 2009, 36, (3), 298–304.

A physics study has been performed to find the optimal application of burnable poison (BP) for an excess reactivity management in a 600 MWth block-type very high temperature reactor. Six potential BP materials (B, Gd, Er, Eu, Sm, Dy) were evaluated for an equilibrium cycle in terms of the major core performance parameters such as the burnup reactivity swing, discharge burnup, fuel and moderator temperature coefficients, and fuel temperature. In addition to the conventional 6-hole BP loading in a fuel block, a 12-hole BP application was also considered in order to accelerate the depletion rate of the BPs. The self-shielding effect of the BP was optimized for a successful management of the excess reactivity by changing the effective diameter of the BP region. Additionally, a mixed BP application of Gd and Er was proposed to make better use of the two BP materials in terms of the reactivity swing and the core temperature coefficients. It has been demonstrated that the burnup reactivity swing over a long cycle period can be reduced from ~15,000 pcm to 3000–5000 pcm with only a small reduction of the discharge fuel burnup.

10/00130 Correlation of submicron dust production in DIII-D to impulsive wall heating from ELMs

Bray, B. D. *et al. Journal of Nuclear Materials*, 2009, 390–391, 96–99.

Submicron dust particles are observed by Rayleigh/Mie scattering from ND:YAG laser light during plasma discharges at DIII-D. The observed dust density decreases gradually over the tokamak major radius in the scrape off layer (SOL) ($1.0 < \Psi < 1.2$ for typical discharges) to the plasma edge. There is a significant increase in dust density with ELMy H-mode discharges relative to L-mode and ELM-free H-mode discharges. The dust density in ELMy H-mode discharges is sensitive to many parameters including the pedestal temperature and ELM frequency and can increase as much as a factor of two with pedestal temperature for similar pedestal pressure and injected power. Dust density decreases with increasing ELM frequency compared to shots with similar stored energy and less frequent ELMs. These measurements suggest the particles are created by impulsive heating from ELMs and the dust density is less sensitive to steady heat flux to the wall.

10/00131 Estimation of the common cause failure probabilities of the components under mixed testing schemes

Kang, D. I. *et al. Annals of Nuclear Energy*, 2009, 36, (3), 493–497.

For the case where trains or channels of standby safety systems consisting of more than two redundant components are tested in a staggered manner, the standby safety components within a train can be tested simultaneously or consecutively. In this case, mixed testing schemes, staggered and non-staggered testing schemes, are used for testing the components. Approximate formulas, based on the basic parameter method, were developed for the estimation of the common cause failure (CCF) probabilities of the components under mixed testing schemes. The developed formulas were applied to the four redundant check valves of the auxiliary feed water system as a demonstration study for their appropriateness. For a comparison, the CCF probabilities of the four redundant check valves were estimated for the mixed, staggered, and non-staggered testing schemes. The CCF probabilities of the four redundant check valves for the mixed testing schemes were estimated to be higher than those for the staggered testing scheme, and lower than those for the non-staggered testing scheme.

10/00132 Estimation of the fast neutron fluence at control rod tips using a 3-D diffusion/2-D transport multi-step calculation scheme

Ferroukhi, H. *et al. Annals of Nuclear Energy*, 2009, 36, (3), 286–291.

This paper presents the development and application of a methodology to estimate, using conventional deterministic lattice/core analysis methods, the fast neutron fluence at the tips of control rods inserted during operation in PWR reactors. The developed methodology is based on a 3-D Nodal Diffusion/2-D Lattice Transport multi-step calculation scheme, in which the operating history of the nuclear environment around the tip is tracked in 3-D core follow analyses and used thereafter to provide boundary conditions for 2-D transport calculations to compute the fast neutron flux. In subsequent steps, radial and axial correction factors, both based on fast flux results from the 3-D core simulator, are applied to the calculated 2-D transport flux in order to take into account radial leakage effects as well as axial flux gradients around the tip. The fluence is finally estimated through a time-integration of the corrected 2-D transport fast flux. The developed methodology has been applied to estimate the fluence for a total of 15 control rods, over 21 operating cycles of a Swiss nuclear power plant.

10/00133 Fuel retention in tokamaks

Loarer, T. *Journal of Nuclear Materials*, 2009, 390–391, 20–28.

Tritium retention constitutes an outstanding problem for ITER operation and future fusion reactors, particularly for the choice of the first wall materials. In present day tokamaks, fuel retention is evaluated by two complementary methods. The *in situ* gas balance allows evaluation of how much fuel is retained during a discharge and, typically, up to one day of experiments. Post-mortem analysis is used to determine where the fuel is retained, integrated over an experimental campaign. In all the carbon clad devices, using the two methods, the retention is demonstrated to be very closely related to the carbon net erosion. This results from plasma–wall interaction with ion and charge-exchange fluxes, ELMs and is proportional to the pulse duration. The fuel retention by implantation saturates at high wall temperatures and limits the D/C ratio in the deposited layers but, as far as a carbon source exists, the dominant retention process remains the co-deposition of carbon with deuterium. In full metallic device, in the absence of wall conditioning with boron, co-deposition is strongly reduced and fuel retention below 1% can be achieved. Extrapolation to ITER shows that removing the carbon from the plasma-facing components would increase the number of discharges to 2500 before reaching the maximum tritium limit of 700 g.

10/00134 Gas fueling system in LHD

Miyazawa, J. *et al. Fusion Engineering and Design*, 2009, 83, (2–3), 265–268.

Gas fueling is the basic method of plasma density control for thermonuclear fusion devices. It outperforms other fueling methods with respect to ease of steady state operation by density feedback control, ease of handling, low costs for both construction and maintenance, and flexibility in working gas selection. The gas fueling system of the Large Helical Device (LHD) is composed of gas cylinders, gas purifiers, gas reserve tanks, vacuum pumps, and pressure gauges. Hydrogen, helium, neon (or methane), argon, and xenon (or krypton, or helium-3) are regularly filled in the gas reserve tanks. These gases are injected to the vacuum vessel through ‘mass flow controllers (MFCs)’ and/or ‘piezo-electric valves (PVs)’. The MFC feedback controls the flow rate to the preordered value. The PV is driven by preprogrammed mode or density feedback mode. The flow rates of PVs are calibrated *in situ*. All components in the system are directly controlled by a programmable logic controller, which is connected to a private local area network. Users can control the system from personal computers through the network. The graphical user interface for system control and that for setting waveforms to drive PVs are working on MS Windows.

10/00135 Micro/nano scale modification of plasma facing components in LHD and its impact on the metal dust generations

Tokitani, M. *et al. Journal of Nuclear Materials*, 2009, 390–391, 205–869.

First walls and divertor plates of large helical devices (LHDs) are made of stainless steels and isotropic graphite, respectively. They are bombarded by energetic plasma particles, and are caused the radiation damages. For understanding of long-term irradiation effects of metallic first walls, probe specimens of Mo were mounted on the special sample stage of outer-port of the LHD torus which is located at about 2500 mm from LCFS (last closed flux surface) of heliotron plasma, and then, exposed to plasma discharges through the single experimental campaign. Majority of discharge gas was hydrogen or helium. Amorphous re-deposition layer of about few nm thick and large sized blisters with few micrometer were formed at the specimen surface. Formation of dense gas bubbles (1–2 nm), dislocation loops and surface roughening were simultaneously occurred in the sub-surface layer about 30 nm thick. Such nanoscale damages may be mainly caused by helium particle bombardment.

10/00136 Optimization of PWR fuel assembly radial enrichment and burnable poison location based on adaptive simulated annealing

Rogers, T. *et al. Nuclear Engineering and Design*, 2009, 239, (6), 1019–1029.

The focus of this paper is to present a concurrent optimization scheme for the radial pin enrichment and burnable poison location in PWR fuel assemblies. The methodology is based on the Adaptive Simulated Annealing (ASA) technique, coupled with a neutron lattice physics code to update the cost function values. In this work, the variations in the pin U-235 enrichment are variables to be optimized radially, i.e. pin by pin. The authors consider the optimization of two categories of fuel assemblies, with and without Gadolinium burnable poison pins. When burnable poisons are present, both the radial distribution of enrichment and the poison locations are variables in the optimization process. Results for 15 × 15 PWR fuel assembly designs are provided.

10/00137 Overview of the tritium system of Ignitor

Rizzello, C. *et al. Fusion Engineering and Design*, 2009, 83, (4), 594–600.

Among the recent design activities of the Ignitor program, the analysis of the tritium system has been carried out with the aim to describe the main equipments and the operations needed for supplying the deuterium–tritium mixtures and recovering the plasma exhaust. In fact, the tritium system of Ignitor provides for injecting deuterium–tritium mixtures into the vacuum chamber in order to sustain the fusion reaction: furthermore, it generally manages and controls the tritium and the tritiated materials of the machine fuel cycle. Main functions consist of tritium storage and delivery, tritium injection, tritium recovery from plasma exhaust, treatment of the tritiated wastes, detritiation of the contaminated atmospheres, tritium analysis and accountability. In this work an analysis of the designed tritium system of Ignitor is summarized.

10/00138 Progress in lattice Boltzmann methods for magnetohydrodynamic flows relevant to fusion applications

Pattison, M. J. *et al. Fusion Engineering and Design*, 2009, 83, (4), 557–572.

In this paper, an approach to simulating magnetohydrodynamic (MHD) flows based on the lattice Boltzmann method (LBM) is presented. The dynamics of the flow are simulated using a so-called multiple relaxation time (MRT) lattice Boltzmann equation (LBE), in which a source term is included for the Lorentz force. The evolution of the magnetic induction is represented by introducing a vector distribution function and then solving an appropriate lattice kinetic equation for this function. The solution of both distribution functions are obtained through a simple, explicit, and computationally efficient stream-and-collide procedure. The use of the MRT collision term enhances the numerical stability over that of a single relaxation time approach. To apply the methodology to solving practical problems, a new extrapolation-based method for imposing magnetic boundary conditions is introduced and a technique for simulating steady-state flows with low magnetic Prandtl number is developed. In order to resolve thin layers near the walls arising in the presence of high magnetic fields, a non-uniform gridding strategy is introduced through an interpolated-streaming step applied to both distribution functions. These advances are particularly important for applications in fusion engineering where liquid metal flows with low magnetic Prandtl numbers and high Hartmann numbers are introduced. A number of MHD benchmark problems, under various physical and geometrical conditions are presented, including 3-D MHD lid driven cavity flow, high Hartmann number flows and turbulent MHD flows, with good agreement with prior data. Due to the local nature of the method, the

LBM also demonstrated excellent performance on parallel machines, with almost linear scaling up to 128 processors for a MHD flow problem.

10/00139 Recent Canadian advances in nuclear-based hydrogen production and the thermochemical Cu–Cl cycle

Naterer, G. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 2901–2917.

This paper presents recent Canadian advances in nuclear-based production of hydrogen by electrolysis and the thermochemical copper–chlorine (Cu–Cl) cycle. This includes individual process and reactor developments within the Cu–Cl cycle, thermochemical properties, advanced materials, controls, safety, reliability, economic analysis of electrolysis at off-peak hours, and integrating hydrogen plants with Canada's nuclear power plants. These enabling technologies are being developed by a Canadian consortium, as part of the Generation IV International Forum (GIF) for hydrogen production from the next generation of nuclear reactors.

10/00140 Sources: a code for calculating (alpha, n), spontaneous fission, and delayed neutron sources and spectra

Wilson, W. B. *et al. Progress in Nuclear Energy*, 2009, 51, (4–5), 608–613.

SOURCES is a computer code that determines neutron production rates and spectra from (alpha, n) reactions, spontaneous fission, and delayed neutron emission due to the decay of radionuclides in homogeneous media, interface problems, and three-region interface problems. The code is also capable of calculating the neutron production rates due to (alpha, n) reactions induced by a monoenergetic beam of alpha particles incident on a slab of target material. The (alpha, n) spectra are calculated using an assumed isotropic angular distribution in the centre-of-mass system with a library of 107 nuclide decay alpha-particle spectra, 24 sets of measured and/or evaluated (alpha, n) cross sections and product nuclide level branching fractions, and functional alpha particle stopping cross sections for $Z < 106$. Spontaneous fission sources and spectra are calculated with evaluated half-life, spontaneous fission branching, and Watt spectrum parameters for 44 actinides. The delayed neutron spectra are taken from an evaluated library of 105 precursors. The code outputs the magnitude and spectra of the resultant neutron sources. It also provides an analysis of the contributions to that source by each nuclide in the problem.

10/00141 Study of startup transients and power ramping of natural circulation boiling systems

Lakshmanan, S. P. *et al. Nuclear Engineering and Design*, 2009, 239, (6), 1076–1083.

Numerical models of a natural circulation test facility and its prototype have been developed with RELAP5/MOD3.4 code and verified for their grid independence by nodal sensitivity studies. The model of the test facility has been validated for its steady state as well as transient predictions with the help of experimental observations. The transient predictions and parametric trends obtained by the numerical model of the prototype have been compared with those of the numerical model of the test facility. Thus, the ability of RELAP5 code to predict the transients during startup of a natural circulation boiling water reactor is verified. A powering procedure for the test facility has been conceptualized with the help of its RELAP5 model and demonstrated experimentally. Based on this, a similar powering procedure for the prototype has been proposed and simulated numerically with its RELAP5 model.

10/00142 Synchronous Databus Network in ITER: open source real-time network for the next nuclear fusion experiment

Boncagni, L. *et al. Fusion Engineering and Design*, 2009, 83, (2–3), 504–510.

The next nuclear fusion experiment, ITER, is providing the infrastructure for the optimal operation of a burning plasma, requiring feedback control of discharge parameters and on-line evaluation of computationally intensive models running in a cluster of controller nodes. Thus, the synchronization of the available information on the plasma and plant state variables among the controller nodes is a key issue for ITER. The ITER conceptual design aims to perform feedback control on a cluster of distributed controllers connected by a Synchronous Databus Network (SDN). Therefore it is mandatory to achieve a deterministic data exchange among the controller nodes with a refresh rate of at least 1 kHz and a jitter of at least 50 μs. Thus, a conservative estimate of the data flow within the controller network can be 3 kSample/ms. In this paper the open source RTnet project is evaluated to meet the requirements of the SDN of ITER. A testbed involving a cluster of eight nodes connected over a standard ethernet network has been set up to simulate a distributed real-time control system. The main goal of the test is to verify the compliance of the performance with the ITER SDN requirements.

10/00143 The status of the ITER CODAC conceptual design

Lister, J. B. *et al. Fusion Engineering and Design*, 2009, 83, (2–3), 164–169.

CODAC orchestrates the activity of 80–120 plant systems in normal ITER operation using a set of dedicated networks. Interlock systems protect ITER from potentially damaging operating off-normal conditions, using a segregated network. Safety systems protect the personnel and the environment and the nuclear safety systems will be subject to licensing. The principal challenges to be met in the design and implementation of CODAC include: complexity, reliability, transparent access respecting security, a high experiment data rate and data volume since ITER is an experimental reactor, scientific exploitation from multiple participant team experiment sites and the long 35-year-period for construction and operation. Two non-technical challenges drive the CODAC design. Firstly all technical plant systems follow an 'in-kind' procurement model, as opposed to a direct commercial contractual relationship with suppliers. Secondly, the period of procurement will, itself, be long compared with the evolution of technologies in the fields of control and data acquisition. This paper addresses the various phases from definition of procurement agreements through to on-site commissioning of the project.

10/00144 Thermal hydraulic challenges of gas cooled fast reactors with passive safety features

Pope, M. A. *et al. Nuclear Engineering and Design*, 2009, 239, (5), 840–854.

Transient response of a gas cooled fast reactor (GFR) coupled to a recompression supercritical CO_2 (S-CO_2) power conversion system (PCS) in a direct cycle to a loss of coolant accident (LOCA) and a loss of generator load accident is analysed using RELAP5–3D. A number of thermal hydraulic challenges for GFR design are pointed out as the designers strive to accommodate cooling of the high power density core of a fast reactor by a gas with its inherently low heat transfer capability, in particular under post-LOCA events when system pressure is lost and when reliance on passive decay heat removal (DHR) is emphasized. Although it is possible to design a S-CO_2 cooled GFR that can survive LOCA by cooling the core through natural circulating loops between the core and elevated emergency cooling heat exchangers, it is not an attractive approach because of various bypass paths that can, depending on break location, degrade core cooling. Moreover, natural circulation gas loops can operate in deteriorated heat transfer regimes with substantial reduction of heat transfer coefficient: as low as 30% of forced convection values, and data and correlations in these regimes carry large uncertainties. Therefore, reliable battery powered blowers for post-LOCA decay heat removal that provide flow in well-defined regimes with low uncertainty, and can be easily overdesigned to accommodate bypass flows were selected. The results confirm that a GFR with such a DHR system and negative coolant void worth can withstand LOCA with and without scram as well as loss of electrical load without exceeding core temperature and turbomachinery overspeed limits.

10/00145 Thermodiffusion in porous media: multi-domain constituent separation

Bennacer, R. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1725–1733.

A numerical study is carried out on double-diffusive, natural convection within a vertical annular, porous cylinder. The flow is driven by buoyancy force due to an externally applied constant temperature difference on the vertical cylinder while the horizontal surfaces are impermeable and adiabatic. The effects of cross phenomena 'Soret effect' were considered in the analysis. It is demonstrated that the cylindrical annulus permits a higher thermal gradient. It is established that such system has an optimal separation effect for a given thermal Rayleigh number, Ra_T. To overcome such limitation, two sub-domains (buffer) allowing filtration separation was proposed and investigated. The flow field, temperature and concentration distributions are obtained in terms of the governing parameters. The effect of the sub-domains scales, the Darcy number, Da, and the curvature, R, on flow, temperature and species separation ability is found to be significant.

Economics, policy, supplies, forecasts

10/00146 Business risks to utilities as new nuclear power costs escalate

Severance, C. A. *The Electricity Journal*, 2009, 22, (4), 112–120.

A nuclear power megaproject carries with it severe business risks. Despite attempts to shift these risks to taxpayers and ratepayers, ultimately there are no guarantees for utility shareholders. Utility management needs to keep some core principles in mind.

10/00147 Control system for electron cyclotron resonance heating in the large helical device

Kubo, S. *et al. Fusion Engineering and Design*, 2009, 83, (2–3), 256–259.

The configuration of and methods for the electron cyclotron resonance heating (ECRH) control system in the Large Helical Device (LHD) are discussed. The ECRH system is routinely used for high electron temperature plasma production and sustainment in the LHD and must be remotely operated reliably and stably. The ECRH system consists of several elements that require reliable control and monitoring, including gyrotrons, high voltage power supplies, millimeter wave transmission systems, and antenna systems.

10/00148 Deliberately small reactors and the second nuclear era

Ingersoll, D. T. *Progress in Nuclear Energy*, 2009, 51, (4–5), 589–603.

Smaller sized nuclear reactors were instrumental during the pioneering days of commercial nuclear power to facilitate the development and demonstration of early reactor technologies and to establish operational experience for the fledgling nuclear power industry. As the USA embarks on its 'second nuclear era,' the question becomes: Will smaller sized plants have a significant role in meeting the nation's needs for electricity and other energy demands? A brief review of nuclear history is presented relative to plant size considerations, followed by a review of several commonly cited benefits of small reactors. Several 'deliberately small' designs currently being developed in the US are briefly described, as well as some of the technical and institutional challenges faced by these designs. Deliberately small reactors offer substantial benefits in safety, security, operational flexibilities and economics, and they are well positioned to figure prominently in the second nuclear era.

10/00149 Design of the Magnum-PSI safety, control and data acquisition system

van der Linden, G. W. *et al. Fusion Engineering and Design*, 2009, 83, (2–3), 273–275.

The FOM-Institute for Plasma Physics Rijnhuizen has started the construction of Magnum-PSI, a magnetized (3 T), steady-state, large area (80 cm^2) high-flux (up to 10^{24} H^+ions $\mathrm{m}^{-2}\,\mathrm{s}^{-1}$) plasma generator. The aim of this linear plasma device is to provide a controlled, highly accessible laboratory experiment facility in which the interaction of a magnetized plasma with different surfaces can be studied in detail. Magnum-PSI consists of several subsystems including vacuum, cooling, plasma source, target station, and a number of diagnostic systems. The safety, Control, Data Acquisition and Communication (CODAC) system integrates these subsystems and provides an interface for the Magnum-PSI users. The CODAC system is designed in parallel with the Magnum-PSI hardware to maximize compatibility and usability. The CODAC system must handle the step-by-step construction and expansion of the Magnum-PSI system without compromising human and system safety in each step, combine manual and remote control, and provide a central data storage and implement automated experiment execution. Key features of the CODAC system are a layered, modular and distributed design, the use of intelligent devices (e.g. commercial computer controlled cooling units), a centralized data storage built on HDF5, and a communication layer built on ZeroC$^{\mathrm{TM}}$ Ice$^{\mathrm{TM}}$. A significant part of the design is based on existing open source software components, integrated using C and Python code.

10/00150 Development of a thermal–hydraulic analysis code for research reactors with plate fuels

Lu, Q. *et al. Annals of Nuclear Energy*, 2009, 36, (4), 433–447.

The thermal–hydraulic analysis code THAC-PRR has been developed with Visual Fortran 6.5 for the investigation of plate type fuel reactors. It is based on the fundamental conservation of mass, momentum and energy, and proper constitutive correlations for flow friction factor, heat transfer and thermophysical properties. Moreover, a simple and improved lumped-differential method has been adopted to analyse the conjugate heat transfer between the fuel plate and the coolant. The reactivity insertion accident and loss of flow accident, which have been defined in the IAEA 10 MW MTR Benchmark program, were analysed with this developed program for the code-to-code validation. Good agreement was achieved. Furthermore, the accidents due to the partial (95%) and total (100%) blockage of one channel in the IAEA 10 MW MTR were investigated with THAC-PRR. The results showed that if the blockage occurred in the average channel, there was no boiling occurred even the channel was totally obstructed. The reason was that the heat was transferred to the adjacent channels by conduction through the fuel plates, which formed the obstructed channel. However, if the blockage occurred in the hot channel, boiling did occur. This indicated that it is very important to consider the interaction between the blocked channel and the adjacent channels in this type of transient.

10/00151 Development of the supervisory discharge operation monitoring system for JT-60

Sueoka, M. *et al. Fusion Engineering and Design*, 2009, 83, (2–3), 283–286.

For safety and efficient operation of a fusion device, appropriate information should be provided to the personnel participating in the experiment. In a continuing effort to meet this requirement, the authors have recently developed highlight displays showing the plasma movie, the status of the discharge sequence, the discharge schedule, the status of present troubles, etc. These highlight displays are presented on the large (65 in.) TV monitor in front of the central consoles. These displays are automatically changed according to the timing signals of the JT-60 discharge sequence and/or at the JT-60 session leader's request. The authors call this system 'the supervisory discharge operation monitoring system'. This report describes the technical details of both this system and the discharge information management system (DIMS).

10/00152 Does Brazil need new nuclear power plants?

de Carvalho, J. F. and Sauer, I. L. *Energy Policy*, 2009, 37, (4), 1580–1584.

In October 2008, the Brazilian government announced plans to invest US$212 billion in the construction of nuclear power plants, totalling a joint capacity of 60,000 MW. Apart from this program, officials had already announced the completion of the construction of the nuclear plant Angra III; the construction of large-scale hydroelectric plans in the Amazon and the implantation of natural gas, biomass and coal thermoelectric plants in other regions throughout the country. Each of these projects has its proponents and its opponents, who bring forth concerns and create heated debates in the specialized forums. In this article, some of these concerns are explained, especially under the perspective of the comparative analysis of costs involved. Under such merit figures, the nuclear option, when compared to hydro plants, combined with conventional thermal and biomass-fueled plants, and even wind, to expand Brazilian power-generation capacity, does not appear as a priority.

10/00153 Failure of high burnup fuels under reactivity-initiated accident conditions

Sugiyama, T. *et al. Annals of Nuclear Energy*, 2009, 36, (3), 380–385.

Pulse irradiation experiments of high burnup light-water-reactor fuels were performed to assess the fuel failure limit in a postulated reactivity-initiated accident (RIA). A BWR-$\mathrm{UO_2}$ rod at a burnup of 69 GW d/t failed due to pellet-cladding mechanical interaction (PCMI) in the test LS-1. The fuel enthalpy at which fuel failure occurred was comparable to those for PWR-$\mathrm{UO_2}$ rods of 71 to 77 GW d/t with more corroded cladding. Comparison of cladding metallographs between the BWR and PWR fuel rods suggested that the morphology of hydride precipitation, which depends on the cladding texture, affects the fuel failure limit. The tests BZ-1 and BZ-2 with PWR-MOX rods of 48 and 59 GW d/t, respectively, also resulted in PCMI failure. The fuel enthalpies at failure were consistent with a tendency formed by the previous test results with $\mathrm{UO_2}$ fuel rods, if the failure enthalpy is plotted as a function of the cladding outer oxide thickness. Therefore, the PCMI failure limit under RIA conditions depends on the cladding corrosion states including oxidation and hydride precipitation, and the same failure limit is applicable to $\mathrm{UO_2}$ and MOX fuels below 59 GW d/t.

10/00154 Improving SFR economics through innovations from thermal design and analysis aspects

Zhao, H. *et al. Nuclear Engineering and Design*, 2009, 239, (6), 1042–1055.

Achieving economic competitiveness as compared to LWRs and other Generation IV (Gen-IV) reactors is one of the major requirements to attract large-scale investment in commercial sodium cooled fast reactor (SFR) power plants. Advances in R&D for advanced SFR fuel and structural materials provide key long-term opportunities to improve SFR economics. In addition, other new opportunities are emerging to further improve SFR economics. This paper provides an overview on potential ideas from the perspective of thermal hydraulics to improve SFR economics. These include: (1) a new hybrid loop-pool reactor design to further optimize economics, safety, and reliability of SFRs with more flexibility, (2) a multiple-reheat and intercooling helium Brayton cycle to improve plant thermal efficiency and to reduce safety related overnight and operation costs, and (3) modern multi-physics thermal analysis methods to reduce analysis uncertainties and associated requirements for over-conservatism in reactor design. This paper reviews advances in all three areas and their potential beneficial impacts on SFR economics.

10/00155 Italy makes u-turn on nuclear power, but hurdles remain

Anon., *The Electricity Journal*, 2009, 22, (4), 5–6.
Prime Minister Berlusconi's centre-right government envisions nuclear power providing as much as 25% of Italy's electricity but it has not specified by when.

10/00156 Progress of a cost optimization for an HLW repository in Korea

Kim, S. K. *et al. Progress in Nuclear Energy*, 2009, 51, (3), 401–408.
This paper provides the results of a cost optimization for a CANDU spent fuel canister as well as the operational duration of an HLW repository. From the design change of an advanced-CANDU spent fuel canister, the overall costs were expected to be reduced by 124 MEUR in the case of disposing of 36,000 tU in an HLW repository, and it was also found that the optimal operational duration for an HLW repository was 83 years, to minimize the total cost. But this operational duration was only calculated from the aspect of cost benefits with economics' perspectives. The authors confirmed that the canister and operational duration are the dominant cost drivers for surface facilities and underground facilities for a cost optimization, respectively. Especially, the manufacturing method of an outer canister using the cold spray coating technique which was developed through collaboration with a domestic company is suggested to minimize the overall costs.

10/00157 Radionuclide transfer to invertebrates and small mammals in a coastal sand dune ecosystem

Wood, M. D. *et al. Science of the Total Environment*, 2009, 407, (13), 4062–4074.
International intercomparisons of models to assess the impact of ionizing radiation on wildlife have identified radionuclide transfer assumptions as a significant source of uncertainty in the modelling process. There is a need to improve the underpinning data sets on radionuclide transfer to reduce this uncertainty, especially for poorly studied ecosystems such as coastal sand dunes. This paper presents the results of the first published study of radionuclide transfer to invertebrates and small mammals in a coastal sand dune ecosystem. Activity concentrations of ^{137}Cs, ^{238}Pu, $^{239+240}$Pu and ^{241}Am are reported for detritivorous, herbivorous, carnivorous and omnivorous biota. Differences in activity concentrations measured in the sand dune biota are related to the trophic level of the organisms and the influence of sea-to-land transfer is apparent in the food chain transfer observed at the site. There are notable differences in the concentration ratios (CRs) calculated for the sand dune biota compared to other terrestrial ecosystems, especially for the small mammals which have CRs that are two orders of magnitude lower than the generic terrestrial ecosystem CRs published by the recent EC EURATOM ERICA project. The lower CRs at the sand dunes may be due to the influence of other cations from the marine environment (e.g. K and Na) on the net radionuclide transfer observed, but further research is required to test this hypothesis.

10/00158 The exciting journey of designing an advanced reactor

Carelli, M. D. *Nuclear Engineering and Design*, 2009, 239, (5), 880–887.
This article chronicles the development of International Reactor Innovative and Secure (IRIS) from its inception to the present. Rather than being a discussion of the reactor design and its characteristics, the focus is on how the project has progressed, the design alternatives that have been considered and the rationale behind the final choices. It provides an insider's view how an idea has evolved over the years into a full-fledged design of an advanced nuclear reactor.

10/00159 Towards a better understanding of iodine chemistry in RCS of nuclear reactors

Girault, N. *et al. Nuclear Engineering and Design*, 2009, 239, (6), 1162–1170.
The Phebus FP in-reactor integral experiments provided new insights into iodine transport through the primary circuit. Indeed, in these tests transported iodine was often found not associated with caesium as generally postulated up to now. Several iodine species were experimentally shown to have been transported in the hot leg at 700 °C, while a fraction was also suspected to be in a gaseous form in the cold leg at 150 °C. For a better estimate of the iodine source term to the containment, both in terms of speciation and quantity, it becomes thus necessary to reconsider iodine species behaviour along their pathway in the reactor coolant system (RCS). This paper presents the current understanding, mainly based on SOPHAEROS equilibrium chemistry calculations of Phebus FP tests performed within the I-RCS technical circle of the SARNET network of excellence in the EU 6th Framework programme. The suspected connection existing between Cs, Mo, Cd and I chemistry and the strong influence of both their release kinetics and related species thermodynamic properties on the iodine speciation in different environments (reducing/oxidizing) are highlighted. Potential explanations for the predicted iodine volatility and the level of association of I to Cs are also discussed.

10/00160 VVER vessel steel corrosion at interaction with molten corium in oxidizing atmosphere

Bechta, S. V. *et al. Nuclear Engineering and Design*, 2009, 239, (6), 1103–1112.
The long-term in-vessel corium retention (IVR) in the lower head bears a risk of the vessel wall deterioration caused by steel corrosion. The ISTC METCOR Project has studied physicochemical impact of prototypic coria having different compositions in air and steam and has generated valuable experimental data on vessel steel corrosion. It is found that the corrosion rate is sensitive to corium composition, but the composition of oxidizing above-melt atmosphere (air, steam) has practically no influence on it. A model of the corrosion process that integrates the experimental data, is proposed and used for development of correlations.

06 ELECTRICAL POWER SUPPLY AND UTILIZATION

Scientific, technical

10/00161 A new IEEE Std 1459–2000 – compatible time-domain formulation for apparent power

de Almeida, J. E. L. *et al. Electric Power Systems Research*, 2009, 79, (4), 505–510.
This paper presents the development of new time-domain equations related to the definition of apparent power. These equations are compatible with the IEEE Std 1459–2000 Standard. When the application of these formulations involves an adequate quantity of samples, thus obeying the Nyquist criterion, they can be utilized without restrictions regarding distortion, imbalance and asymmetry. Thus, they may be used in numeric meters for power measurements. In addition, unlike the above-mentioned standard, they do not oversimplify with respect to the phase and neutral resistance ratio or the percentage of delta-connected and wye-connected loads. This paper uses these formulations to present several illustrative examples regarding the apparent power definition. Simulated cases have confirmed that both approaches, American and European, lead to similar results, which differ only if the voltage homopolar component is present.

10/00162 A new methodology for identification of critical lines using damping sensitivity analysis

Cho, Y.-S. *et al. Electric Power Systems Research*, 2009, 79, (4), 562–568.
When an inter-area mode dominates a low-frequency oscillation in a stressed condition, control of the active power flow of interface lines, with compensating devices, can effectively reduce the electromechanical power oscillations. In general, interface lines in which inter-area oscillations are large are considered to be good locations for installation of compensating devices. A sensitivity analysis with respect to change in active power flow can provide an important factor in electric power system operation. This paper proposes a new methodology to calculate the damping sensitivity with respect to change in active power flow, which can be useful for accurate selection of critical lines from the viewpoint of small-signal stability. In the proposed methodology, a damping sensitivity index is used to select the critical lines to damp power system oscillations. This paper describes how to derive the damping sensitivity for the selected mode and illustrates an example applying the proposed algorithm to a simple two-area system and the New England 39-bus test system.

10/00163 A review on advances in alkali metal thermal to electric converters (AMTECs)

Wu, S.-Y. *et al. International Journal of Energy Research*, 2009, 33, (10), 868–892.
The alkali metal thermal to electric converter (AMTEC) is one of the most promising technologies for direct conversion of thermal energy to electricity and has been receiving attention in the field of energy

conversion and utilization in the past several decades. This paper aims to present a comprehensive review of the state of the art in the research and development of the AMTEC, including its working principles and types, historical development and applications, analytical models, working fluids, electrode materials, as well as the performance and efficiency improvement. The current two major problems encountered by the AMTEC, the time-dependent power degradation and relatively low efficiency compared to its theoretical value, are discussed in depth. In addition, a brief comparison of the AMTEC with other direct thermal to electric converters (DTECs), such as the thermoelectrics converter (TEC), thermionics converter, and thermophotovoltaics converter, is given, and combinations of different DTECs to further improve DTECs' power generation and overall conversion efficiency are demonstrated. Future research and development directions and the issues that need to be further investigated are also suggested. It is believed that this comprehensive review will be beneficial to the design, simulation, analysis, performance assessment, and applications of various types of AMTECs.

10/00164 Design and analysis of a thermal hydraulic integral test facility for Bushehr nuclear power plant

Khoshnevis, T. R. *et al. Progress in Nuclear Energy*, 2009, 51, (3), 443–450.

In this paper, design and analysis of a thermal hydraulic integral test facility for Bushehr Nuclear Power Plant (NPP) is presented. The Bushehr Integral Test Facility (BITF) is a test facility designed to model the thermal-hydraulic behaviours of the Bushehr NPP (VVER-1000) pressurized water reactors currently in use in IRAN. These reactors have unique features that differ from other PWR designs. The BITF simulates the major components and systems of the reference NPP, making it possible to examine postulated small and medium break a loss of coolant accidents (LOCAs) and operational transients. The BITF is a volume-scaled model (1:1375). To ensure that gravitational forces remain equal to those in the reference reactor, the major components and systems in the BITF preserve 1:1 elevation equivalence to the reference reactor. The facility has four loops (each one consists of a hot leg, a steam generator, a loop seal, a main circulation pump and a cold leg), a pressurizer connected via two surge line to the hot leg of the loops 2, 4, the emergency-core-cooling system (ECCS) which is provided by an active pump simulating high and low pressure injection systems, and four hydro-accumulators. The report also contains a comparison between experimental data of PSB test facility and RELAP5 calculations of BITF facility under steady state condition of the reactor power 15% from the nominal.

10/00165 Development of an economical model to determine an appropriate feed-in tariff for grid-connected solar PV electricity in all states of Australia

Zahedi, A. *et al. Renewable and Sustainable Energy Reviews*, 2009, 13, (4), 871–878.

Australia is a country with a vast amount of natural resources including sun and wind. Australia lies between latitude of 10–45°S and longitude of 112–152°E, with a daily solar exposure of between less than 3 MJ/(m^2 day) in winter and more than 30 MJ/(m^2 day) in summer. Global solar radiation in Australia varies between minimum of 3285 MJ/(m^2 year) in Hobart to 8760 MJ/(m^2 year) in Northern Territory. As a result of this wide range of radiation level there will be a big difference between costs of solar PV electricity in different locations. A study that was recently conducted on the solar PV electricity price in all states of Australia. For this purpose, an economical model and a computer simulation have been developed to determine the accurate unit price of grid-connected roof-top solar photovoltaic (PV) electricity in A$/kWh for all state of Australia. The benefit of this computer simulation is that it is possible to accurately determine the most appropriate feed-in tariff of grid-connected solar PV energy system. While the main objective of this paper is to present the results of this study, a further objective is to present the details of the unit price of solar PV electricity in the state of Victoria in each month and then to compare with electricity price from conventional power systems, which is currently applied to this state. The state Victoria is located south of Australia and in terms of sun radiation is second lowest compared with the other Australian states. The computer simulation developed for this study makes it possible to determine the cost of grid-connected solar PV electricity at any location in any country based on availability of average daily solar exposure of each month as well as economical factors of the country.

10/00166 Exergy analysis of gas turbine trigeneration system for combined production of power heat and refrigeration

Khaliq, A. *International Journal of Refrigeration*, 2009, 32, (3), 534–545.

A conceptual trigeneration system is proposed based on the conventional gas turbine cycle for the high temperature heat addition while adopting the heat recovery steam generator for process heat and vapour absorption refrigeration for the cold production. Combined first and second law approach is applied and computational analysis is performed to investigate the effects of overall pressure ratio, turbine inlet temperature, pressure drop in combustor and heat recovery steam generator, and evaporator temperature on the exergy destruction in each component, first law efficiency, electrical to thermal energy ratio, and second law efficiency of the system. Thermodynamic analysis indicates that exergy destruction in combustion chamber and HRSG is significantly affected by the pressure ratio and turbine inlet temperature, and not at all affected by pressure drop and evaporator temperature. The process heat pressure and evaporator temperature causes significant exergy destruction in various components of vapour absorption refrigeration cycle and HRSG. It also indicates that maximum exergy is destroyed during the combustion and steam generation process; which represents over 80% of the total exergy destruction in the overall system. The first law efficiency, electrical to thermal energy ratio and second law efficiency of the trigeneration, cogeneration, and gas turbine cycle significantly varies with the change in overall pressure ratio and turbine inlet temperature, but the change in pressure drop, process heat pressure, and evaporator temperature shows small variations in these parameters. Decision makers should find the methodology contained in this paper useful in the comparison and selection of advanced heat recovery systems.

10/00167 Improvement of proton exchange membrane fuel cell overall efficiency by integrating heat-to-electricity conversion

Xie, C. *et al. Journal of Power Sources*, 2009, 191, (2), 433–441.

Proton exchange membrane fuel cells (PEMFCs) have shown to be well suited for distributed power generation due to their excellent performance. However, a PEMFC produces a considerable amount of heat in the process of electrochemical reaction. It is desirable to use thermal energy for electricity generation in addition to heating applications. Based on the operating characteristics of a PEMFC, an advanced thermal energy conversion system using 'ocean thermal energy conversion' technology is applied to exploit the thermal energy of the PEMFC for electricity generation. Through this combination of technology, this unique PEMFC power plant not only achieves the combined heat and power efficiency, but also adequately utilizes heat to generate more valuable electricity. Exergy analysis illustrates the improvement of overall efficiency and energy flow distribution in the power plant. Analytical results show that the overall efficiency of the PEMFC is increased by 0.4–2.3% due to the thermal energy conversion (TEC) system. It is also evident that the PEMFC should operate within the optimal load range by balancing the design parameters of the PEMFC and of the TEC system.

10/00168 Integration of a hydraulic production plant in a weak power system on a long radial line

Larivière, P. and Racine, M. *Electric Power Systems Research*, 2009, 79, (3), 460–465.

Integrating power plants on long lines and weak power systems requires some care. To this effect, a study was conducted to determine if severe disturbances could result when a hydraulic production plant is integrated along a very long radial transmission line. Frequency responses were evaluated to identify possible resonant system operating conditions. Many events such as faults, transformer energizing and line opening were investigated. All power plant synchronous machines were represented including exciter and governor regulators. Impact of dynamic modelling of the load was examined. The study demonstrates that the overall protective strategy implemented will limit worst overvoltage constraints imposed to equipment and load within an acceptable level.

10/00169 Methanol decomposition fuel processor for portable power applications

Wilson, M. S. *International Journal of Hydrogen Energy*, 2009, 34, (7), 2955–2964.

A new fuel processor approach for portable fuel cell power sources significantly improves upon microreformers by overcoming the difficulties with heat deficiencies and contaminants in the product hydrogen. Instead of reforming, the processor uses methanol decomposition to enable the byproduct, carbon monoxide (CO), to be used as the heat source. A hydrogen permselective membrane segregates the CO for combustion in an integrated burner, maximizes the decomposition conversion, and provides pure hydrogen for a fuel cell. Discharging the CO-rich retentate through an ejector to draw combustion air into the burner greatly simplifies the system. High and stable hydrogen yields are attained with optimized catalysts and fuel compositions. The resultant simple, efficient, and self-heating processor produces 85% of the hydrogen content of the fuel. A 20 W autonomous power source based on this novel fuel processor demonstrates a fuel energy density $>1.5\,\mathrm{Wh\,g^{-1}}_{(\mathrm{electrical})}$, nearly twice as high as microreformer power sources.

10/00170 Modeling of unified power quality conditioner (UPQC) in distribution systems load flow

Hosseini, M. *et al. Energy Conversion and Management*, 2009, 50, (6), 1578–1585.

This paper presents modelling of unified power quality conditioner (UPQC) in load flow calculations for steady-state voltage compensation. An accurate model for this device is derived for use in load flow calculations. The rating of this device as well as the direction of reactive power injection required to compensate voltage to the desired value (1 p.u.) is derived and discussed analytically and mathematically using the phasor diagram method. Since performance of the compensator varies when it reaches to its maximum capacity, modelling of UPQC in its maximum rating of reactive power injection is derived. The validity of the proposed model is examined using two standard distribution systems consisting of 33 and 69 nodes, respectively. The best location of UPQC for under voltage problem mitigation in the distribution network is determined. The results show the validity of the proposed model for UPQC in large distribution systems.

10/00171 On the appropriate monitoring period for voltage flicker measurement in the presence of distributed generation

Morsi, W. G. and El-Hawary, M. E. *Electric Power Systems Research*, 2009, 79, (4), 557–561.

Voltage flicker or voltage fluctuations are considered a major power quality problem causing temperature rise, generators and motors overloading and affecting humans through the irritating light flicker. It is expected that the level of voltage flicker will increase due to the increased penetration of distributed generation (DG) in the distribution system. Site monitoring is required to make sure that the level of voltage flicker is within the allowed limit. In order to determine the appropriate monitoring period for voltage flicker measurement while considering DGs, two case studies were considered in the paper; 1 week and 1 day monitoring periods. The results reveal that a monitoring period of 1 week may be very long especially in the presence of DG and it may hide valuable information. On the other hand a 1-day monitoring period is more appropriate in these situations. Therefore it is recommended to use 1-day monitoring period instead of 1 week especially in the presence of DG.

10/00172 On-line monitoring of power curves

Kusiak, A. *et al. Renewable Energy*, 2009, 34, (6), 1487–1493.

A data-driven approach to the performance analysis of wind turbines is presented. Turbine performance is captured with a power curve. The power curves are constructed using historical wind turbine data. Three power curve models are developed, one by the least squares method and the other by the maximum likelihood estimation method. The models are solved by an evolutionary strategy algorithm. The power curve model constructed by the least squares method outperforms the one built by the maximum likelihood approach. The third model is non-parametric and is built with the *k*-nearest neighbour (*k*-NN) algorithm. The least squares (parametric) model and the non-parametric model are used for on-line monitoring of the power curve and their performance is analysed.

10/00173 Reactivity control options of space nuclear reactors

Schriener, T. M. and El-Genk, M. S. *Progress in Nuclear Energy*, 2009, 51, (3), 526–542.

This paper compares two ex-core control options of the gas-cooled Submersion Subcritical Safe Space (S ^ 4) reactor with a fast neutrons energy spectrum: (a) rotating BeO drums with 120° thin segments of enriched B_4C in the BeO radial reflector; and (b) sliding segments in the BeO radial reflector. Investigated are the effects on the beginning-of-life (BOL) excess reactivity, reactivity depletion rate and operation life, and the spatial neutron flux distributions and fission power profiles in the core. Also investigated is the effect of reducing the thickness of the enriched B_4C segments in the control drums on the BOL excess reactivity, when one or two of the 6 drums are stuck in the shutdown position. Reducing the thickness of the B_4C segments from 0.5 mm to 0.238 mm, with one drums stuck in the shutdown position, increases BOL cold and hot-clean excess reactivity from +\$1.71 and +\$0.47 to +\$2.38 and +\$0.89, respectively. These reactivity values are almost identical to those of the reactor with one of the six reflector segments stuck open in the shutdown position. Results also showed that the control options made little difference in the reactor performance. The power peaking in the reactor core with sliding reflector segments is slightly lower and the spatial power profiles are relatively flatter. The operation life of the reactor with a sliding reflector segments control, when operating at a nominal thermal power of 471 kW, is only 22 full power days longer than with rotating drums control.

10/00174 Surge voltages and currents into a customer due to nearby lightning

Ametani, A. *et al. Electric Power Systems Research*, 2009, 79, (3), 428–435.

This paper presents the results of an experimental investigation into lightning coming into a house. There are four incoming paths, (1) a low-voltage distribution line (feeder) through a distribution pole, (2) a telephone line, (3) the customer's TV antenna and (4) grounding electrode of a customer's electrical equipment. Based on experimental results, the modelling of each component is explained, and EMTP simulations are carried out. The ground voltage rise is represented by a mutual resistance between grounding electrodes. EMTP simulation results have been observed to agree qualitatively with the measured results, and it becomes possible to investigate lightning surges and current distribution in a customer by an EMTP simulation.

Economics, policy, supplies, forecasts

10/00175 Analysis of market signals in a competitive electricity market using components of network rental

Amarasinghe, L. Y. C. and Annakkage, U. D. *Electric Power Systems Research*, 2009, 79, (4), 635–644.

In the competitive electricity market, locational marginal prices (LMPs) are important pricing signals for the participants as the effects of transmission losses and binding constraints are embedded in LMPs. While these LMPs provide valuable information at each location, they do not provide a detailed description in terms of contributing terms. The LMP components, on the other hand, show the explicit decomposition of LMP into contributing components, and thus, can be considered as better market signals. However, the effects of transmission losses cannot be explicitly seen from the LMP components. In this paper, the components of network rental is proposed to be used as a method in analysing market signals, by decomposing the network rental into contributing components among the consumers. Since, the network rental is the surplus paid by all the consumers, components of network rental show how each consumer has actually overpaid due to losses and each binding constraint separately. A case study is also presented to demonstrate the potential of this proposed method in market signal analysis.

10/00176 Application of the fault tree analysis for assessment of power system reliability

Volkanovski, A. *et al. Reliability Engineering & System Safety*, 2009, 94, (6), 1116–1127.

A new method for power system reliability analysis using the fault tree analysis approach is developed. The method is based on fault trees generated for each load point of the power system. The fault trees are related to disruption of energy delivery from generators to the specific load points. Quantitative evaluation of the fault trees, which represents a standpoint for assessment of reliability of power delivery, enables identification of the most important elements in the power system. The algorithm of the computer code, which facilitates the application of the method, has been applied to the IEEE test system. The power system reliability was assessed and the main contributors to power system reliability have been identified, both qualitatively and quantitatively.

10/00177 Assessment of information impacts in power system security against malicious attacks in a general framework

Bompard, E. *et al. Reliability Engineering & System Safety*, 2009, 94, (6), 1087–1094.

In the analysis of power systems security, recently a new concern related to possible malicious attacks caught much attention. Coordination among different transmission system operators (TSO) in an interconnected power system to counteract such attacks has become an important problem. This paper presents a general framework for describing the physical, cyber and decision-making aspects of the problem and their interrelations; within this framework, an analytic tool for the assessment of information impacts in handling on-line security after a malicious attack is proposed and discussed. The model is based on the socially rational multi-agent systems and the equilibrium of a fictitious play is considered to analyse the impacts of various levels of information available to the interconnected system operators on the outcomes of the decision-making process under attack. A 34-buses test system, with three systems interconnected by tie-lines, is presented to illustrate the model and compare the impacts of different information scenarios.

10/00178 Capital market response to emission rights returns: evidence from the European power sector

Veith, S. *et al. Energy Economics*, 2009, 31, (4), 605–613.

Prior studies on the distributional effects of the European Union's emission trading scheme (EU ETS) have so far only relied on supply and demand data. Empirical evidence from capital markets has been missing. The authors address this gap and measure the ETS's economic consequences, using the expectations of investors towards the regulatory impact on firm value. Employing a multifactor model, it is shown that returns on common stock of the largest affected industry, power generation, are positively correlated with rising prices for emission rights. This implies that the market predicts that firms are not only able to pass on their share of the regulatory burden to customers but even achieve windfall profits by overcompensating for the costs.

10/00179 Contingency constrained economic load dispatch using improved particle swarm optimization for security enhancement

Baskar, G. and Mohan, M. R. *Electric Power Systems Research*, 2009, 79, (4), 615–621.

This paper presents a contingency constrained economic load dispatch (CCELD) using proposed improved particle swarm optimization (IPSO), conventional particle swarm optimization (PSO), evolutionary programming (EP) techniques such as classical EP (CEP), fast-EP (FEP) and mean of classical and fast EP (MFEP) to alleviate line overloading. Power system security enhancement deals with the task of taking remedial action against possible network overloads in the system following the occurrences of contingencies. Line overload can be removed by means of generation redispatching. In the proposed improved PSO, a new velocity strategy equation with scaling factor is proposed and the constriction factor approach (CFA) utilizes the eigenvalue analysis and controls the system behaviour. The CCELD problem is a twin objective function viz. minimization of fuel cost and minimization of severity index. This proposed IPSO-based CCELD approach generates higher quality solution in terms of optimal cost, minimum CPU time and minimum severity index than the other methods. Simulation results on IEEE-118 bus and IEEE-30 bus test systems are presented and compared with the results of other approaches.

10/00180 Cost benefit analysis of a photovoltaic-energy storage electrification solution for remote islands

Kaldellis, J. K. *et al. Renewable Energy*, 2009, 34, (5), 1299–1311.

A large number of various sized islands are spread throughout the south-east Mediterranean Sea. Most of these small islands face serious infrastructure problems, like the insufficient power supply and the low quality of electricity available at very high production cost. In an attempt to improve the life quality of all these isolated communities, an investigation concerning the financial viability of an integrated electrification solution based on one or more photovoltaic generators and an appropriate energy storage system is described. The main target of a similar solution is to maximize the contribution of the photovoltaic generator and minimize the life-cycle electricity generation cost of the remote island networks investigated. In addition, special emphasis is given in order to select the most cost-efficient energy storage configuration available. According to the results obtained for high and medium–high solar potential regions, the proposed configuration is found to be more cost-effective than the existing thermal power stations. Several side benefits like the improved electrical network reliability and the minimization of the environmental and macro-economic impacts resulting from the replacement of the imported oil should also be considered.

10/00181 Global and local effects of decentralised electric power generation on the grid in the Western Balkan Countries (WBC)

Lehner, J. and Weißbach, T. *Energy*, 2009, 34, (5), 555–563.

In the European countries renewable and decentralized electric power generation is continuously gaining in importance. More than one half of the total worldwide installed capacity of wind power plants is located in Europe. Furthermore the electric power generation of small hydro power plants and biomass fired cogeneration plants increases steadily, not least encouraged by legislation. However, especially during off-peak load conditions, a high penetration by decentralized electric power generation can cause significant problems for a stable power system operation and establishes new responsibilities for system operators. A EU-Project has been initiated to investigate the development of renewable energy sources especially for the Western Balkan Countries (WBC), including an analysis of the impact on the grid. The effects of decentralized electric power generation on the grid of the WBC are analysed, aiming for the development of a general methodology to identify critical system configurations. The limits of the feed-in into the existing transmission and distribution systems of decentralized power generation units, not taking part in power system control services, are analysed for steady state conditions. Together with matching approaches of the other project partners, corresponding problems can be addressed already within the planning phase.

10/00182 Global and local emission impact assessment of distributed cogeneration systems with partial-load models

Mancarella, P. and Chicco, G. *Applied Energy*, 2009, 86, (10), 2096–2106.

In this paper, a comprehensive emission assessment framework suitable for addressing distributed cogeneration systems is formulated. Local and global emission impact models are presented to identify upper and lower boundary values of the environmental pressure from pollutants that would be emitted from reference technologies, to be compared to the actual emissions from distributed cogeneration. This provides synthetic information on the relative environmental impact from small-scale CHP sources, useful for general indicative and non-site-specific studies. The emission models are formulated according to an electrical output-based emission factor approach, through which off-design operation and relevant performance are easily accounted for. In particular, in order to address the issues that could arise under off-design operation, an equivalent load model is incorporated within the proposed framework, by exploiting the duration curve of the cogenerator loading and the emissions associated to each loading level. In this way, it is possible to quantify the contribution to the emissions from cogeneration systems that might operate at partial loads for a significant portion of their operation time, as for instance in load-tracking applications. Suitability of the proposed methodology is discussed with respect to hazardous air pollutants such as NO_x and CO, as well as to greenhouse gases such as CO_2. Two case study applications based on the emission data of real microturbines are illustrated in order to highlight the effectiveness of the proposed assessment techniques. The numerical results exemplify the emission impact of distributed cogeneration systems operating under general and realistic loading conditions with respect to average and state-of-the-art conventional technologies.

10/00183 Indications for a changing electricity demand pattern: the temperature dependence of electricity demand in the Netherlands

Hekkenberg, M. *et al. Energy Policy*, 2009, 37, (4), 1542–1551.

This study assesses the electricity demand pattern in the relatively temperate climate of the Netherlands (latitude 52°30′N). Daily electricity demand and average temperature during the period from 1970 until 2007 are investigated for possible trends in the temperature dependence of electricity demand. It is hypothesized that the increased use of cooling applications has shifted the temperature dependence of electricity demand upwards in summer months. The results show significant increases in temperature dependence of electricity demand in May, June, September, October and during the summer holidays. During the period studied, temperature dependence in these months has shifted from negative to positive, meaning that a higher temperature now leads to an increased electricity demand in these months, rather than a decreased demand as observed historically. Although electricity demand in countries with moderate summer temperatures such as the Netherlands generally peaks in winter months and shows a minimum in summer months, this trend may signal the development of an additional peak in summer, especially given the expected climatic change. As power generating capacity may be negatively influenced by higher temperatures due to decreasing process cooling possibilities, an increasing electricity demand at higher temperatures may have important consequences for power generation capacity planning and maintenance scheduling.

10/00184 Long-term trends of electric efficiencies in electricity generation in developing countries

Maruyama, N. and Eckelman, M. J. *Energy Policy*, 2009, 37, (5), 1678–1686.

This analysis provides time-series data on electric efficiencies for 138 countries and regions, covering all fossil fuels for the period 1971–2005, with an emphasis on non-organization for economic cooperation and development (OECD) countries. Fossil fuel consumption for electricity generation in non-OECD countries now exceeds that in the OECD. The historical performance of the top five non-OECD consumers of each fossil fuel for which reliable data are available is presented and discussed. For each fuel, the countries that lead the world in efficiency are used for benchmarks; bringing the rest of the world up to these standards would result in energy savings of 26 EJ (equivalent to 5% of global energy consumption) and CO_2 emissions reduction of 2.1 Pg (equivalent to 8% of global CO_2 emissions). Coal showed the largest potential margin of improvement for both energy and CO_2, with possible savings equivalent to 3% of current global energy consumption and 5% of global CO_2 emissions. The gap in electric efficiency between OECD and non-OECD countries over the past 35 years has widened for coal-fired generation, stayed relatively constant for natural gas, but has shrunk for petroleum. The results show the very gradual nature of overall efficiency improvements and the significant differences among regions and countries.

10/00185 Multi-objective market clearing of joint energy and reserves auctions ensuring power system security

Aghaei, J. *et al. Energy Conversion and Management*, 2009, 50, (4), 899–906.

A model and solution approach to day-ahead market clearing of joint energy and reserves auctions is proposed in this paper. The model represents the clearing system used by ISO in charge of both the market operation and system security. A multiobjective mathematical programming (MMP) formulation is implemented for provision of ancillary services (automatic generation control or agc, spinning, non-spinning and operational reserves) as well as energy in simultaneous auctions by pool-based aggregated market scheme. System security is taken into account in the market clearing procedure as the extra objective functions of the optimization problem. So, in the MMP formulation of the market clearing process, the objective functions (generation cost and security indices) are optimized while meeting AC power flow constraints, system reserve requirements and lost opportunity cost (LOC) considerations. The model is applied to the IEEE 24-bus reliability test system (IEEE 24-bus RTS), and simulation studies are carried out to examine the effectiveness of the proposed method.

10/00186 On the temperature dependence of photovoltaic module electrical performance: a review of efficiency/power correlations

Skoplaki, E. and Palyvos, J. A. *Solar Energy*, 2009, 83, (5), 614–624.

A brief discussion is presented regarding the operating temperature of one-sun commercial grade silicon-based solar cells/modules and its effect upon the electrical performance of photovoltaic installations. Suitable tabulations are given for most of the known algebraic forms which express the temperature dependence of solar electrical efficiency and, equivalently, solar power. Finally, the thermal aspects of the major power/energy rating methods are briefly discussed.

10/00187 Pathways for the North European electricity supply

Odenberger, M. *et al. Energy Policy*, 2009, 37, (5), 1660–1677.

This paper investigates the development of the electricity-supply systems in Northern Europe (Germany, UK, Denmark, Finland, Sweden and Norway) until the year 2050. The focus is on the response to an assumed common stringent CO_2-reduction target and on the role of carbon capture and storage (CCS) technologies. Special emphasis is put on turn-over in capital stock, timing of investments and the infrastructural implications of large-scale introduction of CCS. The analysis is carried out through scenario analysis with the aid of a techno-economic model, in which a case including CCS is compared to a case excluding this option. The phase out of the present capital stock (power plants) is included from the Chalmers energy infrastructure databases, which gives information on present and planned power plants down to block level for plants exceeding 10 MW net electric power. Assuming technical lifetimes for these plants yield residual capacities in each year, here referred to as the phase-out pattern. CCS technologies are assumed to become commercially available in 2020. The age structure of the power plants indicate that full turn-over in capital stock will take several decades with the present generation capacities accounting for around 50% of generated electricity in 2020. The results show that CO_2 emission reductions of 20% and 60% by the years 2020 and 2050, respectively, relative to 1990, can be met at a marginal cost of abatement of about 25–40 €/ton CO_2 over the period studied if CCS is included as an option from 2020. At the same time the marginal cost of generating electricity lies in the range 45–60 €/MWh. Excluding CCS raises the marginal cost of abatement with about 10 €/ton CO_2, whereas the marginal cost of electricity generation increases with roughly 5–10 €/MWh. The CO_2 target by the year 2020 is met by implementation of renewable electricity and fuel shifting from coal to gas. After 2020 CCS technologies constitute an attractive way for cost efficient and almost CO_2-free base load. However, wide-spread application of CCS is an infrastructural challenge with respect to implementing capture plants as well as building up a corresponding CO_2 infrastructure for transportation and storage as well as in coal supply systems. Given the price assumptions applied, gas may not be competitive once CCS enters the system causing early retirements of such units or possibly stranded assets.

10/00188 The analysis of security cost for different energy sources

Jun, E. *et al. Applied Energy*, 2009, 86, (10), 1894–1901.

Global concerns for the security of energy have steadily been on the increase and are expected to become a major issue over the next few decades. Urgent policy response is thus essential. However, little attempt has been made at defining both energy security and energy metrics. In this study, such metrics are provided and apply them to four major energy sources in the Korean electricity market: coal, oil, liquefied natural gas, and nuclear. In the approach, the cost of energy security is measured in terms of supply disruption and price volatility, and the degree of concentration in energy supply and demand is considered using the Hirschman–Herfindahl index. Due to its balanced fuel supply and demand, relatively stable price, and high abundance, nuclear energy is found to be the most competitive energy source in terms of energy security in the Korean electricity market. LNG, on the other hand, was found to have the highest cost in term of energy security due to its high concentration in supply and demand, and its high price volatility. In addition, in terms of cost, it is found that economic security dominates supply security, and as such, it is the main factor in the total security cost. Within the confines of concern for global energy security, the study both broadens the understanding of energy security and enables a strategic approach in the portfolio management of energy consumption.

10/00189 The power of dynamic pricing

Faruqui, A. *et al. The Electricity Journal*, 2009, 22, (3), 42–56.

Using data from a generic California utility, it can be shown that it is feasible to develop dynamic pricing rates for all customer classes. These rates have the potential to reduce system peak demands from 1 to 9 percent.

10/00190 Uncertainties in key low carbon power generation technologies – implication for UK decarbonisation targets

Kannan, R. *Applied Energy*, 2009, 86, (10), 1873–1886.

The UK government's economy-wide 60% carbon dioxide reduction target by 2050 requires a paradigm shift in the whole energy system. Numerous analytical studies have concluded that the power sector is a critical contributor to a low carbon energy system, and electricity generation has dominated the policy discussion on UK decarbonization scenarios. However, range of technical, social and market challenges, combined with alternate market investment strategies mean that large scale deployment of key classes of low carbon electricity technologies is fraught with uncertainty. The UK MARKAL energy systems model has been used to investigate these long-term uncertainties in key electricity generation options. A range of power sector specific parametric sensitivities have been performed under a 'what-if' framework to provide a systematic exploration of least-cost energy system configurations under a broad, integrated set of input assumptions. In this paper results of six sensitivities, via restricted investments in key low carbon technologies to reflect their technical and political uncertainties, and an alternate investment strategies from perceived risk and other barriers, have been presented.

07 STEAM RAISING

Boiler operation/design

10/00191 Application of a neural network based feedwater controller to helical steam generators

Shen, H. and Doster, J. M. *Nuclear Engineering and Design*, 2009, 239, (6), 1056–1065.

In current generation pressurized water reactors (PWRs), the control of steam generator level experiences challenges over the full range of plant operating conditions. These challenges can be particularly troublesome in the low power range where the feedwater is highly subcooled and minor changes in the feed flow may cause oscillations in the SG level, potentially leading to reactor trip. The IRIS reactor concept adds additional challenges to the feedwater control problem as a result of a steam generator design where neither level or steam generator mass inventory can be measured directly. Neural networks have demonstrated capabilities to capture a wide range of dynamic signal transformation and non-linear problems. In this paper a detailed engineering simulation of plant response is used to develop and test neural control methods for the IRIS feedwater control problem. The established neural network mass estimator has demonstrated the capability to predict the steam generator mass under transient conditions, especially at low power levels, which is considered the most challenging region for a full range feed water controller.

10/00192 Constructal steam generator architecture

Kim, Y.S. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (9–10), 2362–2369.

This paper shows that the architecture of a steam generator for a power plant can be deduced on the basis of the constructal law. According to constructal theory, the flow architecture emerges in time such that it provides progressively greater access to its currents. The circulation of water is driven by buoyancy in one large tube (the downcomer) and many parallel smaller tubes (the riser). The total flow volume is fixed. Two flow models are used: single phase liquid in the downcomer and riser, and liquid–vapour mixture in the riser tubes. Features that result from constructal design are: the tube diameters, the number of riser tubes, the water circulation rate, the rate of steam production, and how the flow architecture should change when the operating pressure and the size of the flow system change.

10/00193 Distribution of size in steam turbine power plants

Kim, Y. S. *et al. International Journal of Energy Research*, 2009, 33, (11), 989–998.

This paper shows that the mass inventory for steam turbines can be distributed between high-pressure (HP) and low-pressure (LP) turbines such that the global performance of the power plant is maximal. This is demonstrated for two design classes. For an HP turbine in series with an LP turbine, the optimal intermediate pressure (IP) is a geometric average of HP and LP. The total mass is distributed in a balanced way based on the total mass of turbines. For a train consisting of many turbines expanding the steam at nearly constant temperature, the pressure ratio between consecutive IP should be constant, and more mass should be distributed at HPs. This approach to discovering the configuration of the power plant should be used in conjunction with classical approaches that account for vibration, centrifugal force and blade length.

10/00194 Integrity assessment of an embrittled steam turbine casing

Cheong, K. and Karstensen, A. D. *International Journal of Pressure Vessels and Piping*, 2009, 86, (4), 265–272.

This work reviews a recent structural integrity assessment carried out on a high-pressure turbine inner casing that had suffered from temper embrittlement. The assessment was carried out to demonstrate that the casing can be safely returned to service based on revised operating conditions with particular emphasis on the control of temperature ramp rates during start-up and shutdown events. A retirement-for-cause philosophy was adopted to take into consideration that some operational flexibility will be required prior to the casing being replaced at the next planned outage.

10/00195 Mathematical model of impurities hide out and return in nuclear power plant steam generator

Jahanfarnia, G. and Tashakor, S. *Progress in Nuclear Energy*, 2009, 51, (4–5), 644–648.

This paper discusses a simple mathematical–physical model for describing the dissolved impurities hide out and return phenomenon in the boiling channel, within the viscous sub layer. By solving the equation of convection-diffusion for the liquid phase near the heating surface and the bulk stream, the effect of heat flux in distribution of impurities is considered. With deriving the impurities mass balance based on the presented model and using the impurities mass balance in the viscous sub layer as the boundary conditions, the derived differential equations are solved by the finite volume (upwind) method.

10/00196 Numerical investigation on the flow, combustion and NO_x emission characteristics in a 500 MW_e tangentially fired pulverized-coal boiler

Choi, C. R. and Kim, C. N. *Fuel*, 2009, 88, (9), 1720–1731.

The characteristics of the flow, combustion, temperature and NO_x emissions in a 500 MW_e tangentially fired pulverized-coal boiler are numerically studied using comprehensive models, with emphasis on fuel and thermal NO_x formations. The comparison between the measured values and predicted results shows good agreement, which implies that the adopted combustion and NO_x formation models are suitable for correctly predicting characteristics of the boiler. The relations among the predicted temperature, O_2 and CO_2 mass fractions are discussed based on the calculated distributions. The predicted results clearly show that NO_x formation within the boiler highly depends on the combustion processes as well as the temperature and species concentrations. The results obtained from this study have shown that overfire air (OFA) operation is an efficient way to reduce the NO_x emissions of the pulverized-coal fired boiler. Air staging combustion technology (OFA operation) adopted in this boiler has helped reduce fuel NO_x formation as well as thermal NO_x formation under the present simulated conditions. The decrease in the formation of fuel NO_x is due to the decreased contact of the nitrogen from the fuel with the oxygen within the combustion air, while the decrease in thermal NO_x formation is caused by a decrease in temperature. The detailed results presented in this paper may enhance the understanding of complex flow patterns, combustion processes and NO_x emissions in tangentially fired pulverized-coal boilers, and may also provide a useful basis for NO_x reduction and control.

10/00197 Optimization of pelletisation and combustion in a boiler of 17.5 kW_{th} for vine shoots and industrial cork residue

Mediavilla, I. *et al. Fuel Processing Technology*, 2009, 90, (4), 621–628.

Wood pellets have become an important renewable energy fuel. Nowadays the main raw materials used for their production are wood wastes from wood industries. However, these wood wastes have other uses in Spain and it is necessary to look for other possible raw materials. In this work, vine shoots and industrial cork residue were studied as raw materials. The results showed that pelletization of vine shoots presented a high energy demand. This energy requirement was reduced with the addition of industrial cork residue. Moreover, industrial cork residue decreased the ash content of pellets and increased their heating value, although it decreased their physical properties at the same time. Regarding combustion, the addition of industrial cork residue decreased the accumulation of ash in the pellet burner and its sintering tendency. The major conclusion of the work is that the most appropriate blend to improve pelletization and combustion processes is 30% wt of vine shoots and 70% wt of industrial cork residue.

10/00198 Performance of a direct steam generation solar thermal power plant for electricity production as a function of the solar multiple

Montes, M. J. *et al. Solar Energy*, 2009, 83, (5), 679–689.

This paper describes the influence of the solar multiple on the annual performance of parabolic trough solar thermal power plants with direct steam generation (DSG). The reference system selected is a 50 MW_e DSG power plant, with thermal storage and auxiliary natural gas-fired boiler. It is considered that both systems are necessary for an optimum coupling to the electricity grid. Although thermal storage is an opening issue for DSG technology, it gives an additional degree of freedom for plant performance optimization. Fossil hybridization is also a key element if a reliable electricity production must be guaranteed for a defined time span. Once the yearly parameters of the solar power plant are calculated, the economic analysis is performed, assessing the effect of the solar multiple in the levelized cost of electricity, as well as in the annual natural gas consumption.

10/00199 Potential steam generator tube rupture in the presence of severe accident thermal challenge and tube flaws due to foreign object wear

Liao, Y. and Guentay, S. *Nuclear Engineering and Design*, 2009, 239, (6), 1128–1135.

This study develops a methodology to assess the probability for the degraded PWR steam generator to rupture first in the reactor coolant pressure boundary, under severe accident conditions with counter-current natural circulating high temperature gas in the hot leg and steam generator (SG) tubes. The considered SG tube flaws are caused by foreign object wear, which in recent years has emerged as a major inservice degradation mechanism for the new generation tubing materials. The first step develops the statistical distributions for the flaw frequency, size, and the flaw location with respect to the tube length and the tube's tubesheet position, based on data of hundreds of flaws reported in numerous SG inservice inspection reports. The next step performs thermal-hydraulic analysis using the MELCOR code and recent CFD findings to predict the thermal challenge to the degraded tubes and the tube-to-tube difference in thermal response at the SG entrance. The final step applies the creep rupture models in the Monte Carlo random walk to test the potential for the degraded SG to rupture before the surge line. The mean and range of the SG tube rupture probability can be applied to estimate large early release frequency in probabilistic safety assessment.

10/00200 Two-dimensional modelling of deposits formation on platen superheaters in pulverized coal boilers

Tomeczek, J. and Waclawiak, K. *Fuel*, 2009, 88, (8), 1466–1471.

One-dimensional modelling of deposit formation cannot describe properly the gas and particle flow in the vicinity of heat transfer tubes in boilers. This is especially true of the recirculation zones in the down-stream side of tubes, which cannot be reproduced. The most important information needed is the shape and size of deposits, as this enables heat transfer abatement with boiler operation time to be predicted. This study presents two-dimensional modelling of deposits on platen superheaters in pulverized coal boilers. Tube spacing in industrial boilers was reproduced by the model, in which the particle size dependence of the ash sticking probability was proposed. It was been demonstrated that ash particle size plays an important role in deposit growth mechanisms.

08 COMBUSTION

Burners, combustion systems

10/00201 Activated air plasma flow generated by pulsed arc discharge for combustion enhancement

Nishiyama, H. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1778–1785.

Important operating parameters, temperature characteristics and radical production in an air plasma flow generated by a low-power pulsed arc discharge were experimentally clarified for lean combustion enhancement and surface treatment. Furthermore, the time-dependent thermofluid field downstream from the torch was also clarified numerically and the downstream temperature well agreed with experimental data. Finally, the time evolution of production and decay of the chemical species in air plasma were clarified numerically under a high electric field.

10/00202 An experiment on the effect of oxygen content and air velocity on soot formation in acetylene laminar diffusion flame produced in a burner with a parallel annular coaxial oxidizer flow

Santos, A. Á. B. *et al. International Communications in Heat and Mass Transfer*, 2009, 36, (5), 445–450.

The effect of oxygen content and of the combustion air velocity on soot formation was studied in acetylene diffusion flames. These flames were produced in a burner with a parallel annular coaxial flow of oxidizer. The effect on the flame axial temperature profile was also evaluated. The soot volume fraction was calculated by the laser light extinction methodology. The oxygen content in the combustion air was smaller than 30%, which does not require significant retrofit of existent equipment when the combustion conditions are varied. The results suggest that the parallel manipulation of the oxygen content and of the oxidizer velocity can provide means for managing soot formation and distribution. The formation of soot in industrial combustion systems is of interest in engineering, because the presence of soot in the flame enhances the heat transfer from the combustion gases by thermal radiation, increases the need for burner maintenance, and constitutes an environmental problem when emitted in the atmosphere.

10/00203 Characterization of the porous structure of cokes produced from the blends of three Polish bituminous coking coals

Krzesińska, M. *et al. International Journal of Coal Geology*, 2009, 78, (2), 169–176.

Three Polish coals of varying rank (82.7, 86.2 and 88.7 wt% carbon content) and caking ability (weak, moderate, and strong) were used for the preparation of binary and ternary blends. Many cokes of various internal structure were produced from these blends using a laboratory-scale Jenkner furnace. The bulk porosity and the specific surface area were determined for the resultant cokes using a helium gas displacement pycnometer and the measurements of nitrogen adsorption at −196 °C, respectively. Pores in cokes were observed using optical microscopy. Structure of pore solid walls was studied with TEM. The bulk porosity, the specific surface area and the coke reactivity to CO_2 (*CRI*) were discussed in relation to strongly caking coal concentration in a blend, i.e. to the Zofiówka coal content ranged from 0 to 100% with steps generally, equal to 10%. The *CRI* was found to be exactly linear function (correlation coefficient equal to 0.96), while the specific surface area was approximately linear (correlation coefficient equal to 0.5) dependent on content of the strongly caking coal in a blend. The bulk porosity was almost independent on a blend composition. The *CRI* was found to be additive, dependent on the *CRI* of the cokes obtained from the individual coals used in a blend and the blend composition, unlike the parameters of porous structure of cokes. The *CRI* increased with increasing the specific surface area, but this dependence was not exactly linear. it was suggested therefore that the chemical structure of a solid phase of porous cokes plays an important role in reactivity to gases, not less than that of internal surface area. Cokes with greater molecular orientated domains in solid walls were found to be less reactive to CO_2.

10/00204 Combustion of hydrogen–air in catalytic micro-combustors made of different material

Zhou, J. *et al. International Journal of Hydrogen Energy*, 2009, 34, (8), 3535–3545.

Micro-combustors have low stability, thus catalyst is applied to improve it. In this experiment, the performances of catalytic micro-combustors made of different materials (quartz glass, alumina ceramic, copper) are compared. Asbestine threads are used as the catalyst supports of Pt, and installed in the combustors. According to the experimental results, the combustors have high stability, they keep working until the extreme equivalence ratio close to 0. The stability limits of homogeneous reaction in the quartz glass and alumina ceramic combustor range from 0.0907 to 8.69 and 0.158 to 7.31 on average, respectively. But the two combustors exhibit obvious hot spots, which are 1058 and 728 K at 0.2 L/min, respectively. Whereas the copper combustor has low and uniform temperature distribution on its surface. Moreover, the heat loss in the quartz glass combustor is 4.13 W higher than in the copper one at 0.2 L/min, which is opposite to the conventional situation that heat loss increases with the wall thermal conductivity. Computational fluid dynamic simulation reveals that the reaction modes inside the combustors differ. The higher wall thermal conductivity makes the heterogeneous reaction dominate, thus induces the temperature distribution and heat loss aforementioned.

10/00205 Direct numerical simulation of hydrogen addition in turbulent premixed Bunsen flames using flamelet-generated manifold reduction

Vreman, A. W. *et al. International Journal of Hydrogen Energy*, 2009, 34, (6), 2778–2788.

Direct numerical simulations of a lean premixed turbulent Bunsen flame with hydrogen addition have been performed. The authors show the results for a case with equivalence ratio of 0.7 and a molar fractional distribution of 40% H_2 and 60% CH_4. The flamelet-generated manifold technique is used to reduce the chemistry; flamelets with different equivalence ratios and inflow temperature are used to account for stretch effects that are enhanced by preferential diffusion. The three-dimensional simulation clearly shows enhanced burning velocity in regions convex toward the reactants and reduced burning velocity with possible extinction in regions concave toward the reactants. To obtain these effects it was found to be necessary to include two three-dimensional transport equations with essentially different diffusivities. This point is illustrated by comparison of the results with cases in which either a single transport equation was used or two transport equations with minor differences in diffusivities were used. These latter cases incorporated preferential diffusion in the one-dimensional flamelets (and thus in the manifold), but not in the three-dimensional transport. Thus the three-dimensional preferential diffusion effects are shown to enhance curvature and thereby to increase the turbulent burning velocity and reduce the mean flame height. In addition the turbulent burning velocity increases because hydrogen addition leads to a larger laminar flamelet consumption speed. To demonstrate this second effect, results of the cases mentioned above are compared to the results of simulations of the Bunsen flame with 0% hydrogen added to the fuel.

10/00206 Gas and soot products formed in the pyrolysis of acetylene–ethanol blends under flow reactor conditions

Esarte, C. *et al. Fuel Processing Technology*, 2009, 90, (4), 496–503.

The present paper reports a laboratory study on the pyrolysis of different blends containing acetylene, known as an important soot precursor, and ethanol, regarded as an appropriate additive to conventional fuels aiming to diminish the emission of pollutants coming from combustion processes. Pyrolysis experiments of acetylene–ethanol blends, for a total initial concentration of reactants of 50,000 ppm, with variable volume percentages of ethanol between 0 and 40% with respect to the total concentration of reactants, have been carried out in a quartz flow reactor working in a temperature range of 975–1475 K. The influence of both pyrolysis temperature and ethanol concentration in the blend on the gas and solid products has been evaluated. As the reaction temperature is increased, the soot production is higher and yield to carbonaceous gas products decreases. It is noticed that the presence of ethanol inhibits the production of soot and the diminution of soot formation does not present a linear dependency with the ethanol concentration; the influence is comparatively stronger when adding small amounts of ethanol. The analysis of the gas products reveals that increasing the ethanol percentage in the blend causes an increase of the concentration of some intermediates such as ethylene, ethane, methane or benzene, pointing to a variation of the reacting species which could prevent soot formation. A literature detailed gas phase kinetic mechanism including reaction subsets for acetylene and ethanol conversion has been used to simulate the experimental results. This theoretical study has been carried out with the purpose of analysing the trends of the evolution of gas products and getting a better understanding of the gas phase processes involved in the pyrolysis of the different blends, although soot formation is not included.

10/00207 HCCI experiments with gasoline surrogate fuels modeled by a semidetailed chemical kinetic model

Andrae, J. C. G. and Head, R. A. *Combustion and Flame*, 2009, 156, (4), 842–851.

Experiments in a homogeneous charge compression ignition (HCCI) engine have been conducted with four gasoline surrogate fuel blends. The pure components in the surrogate fuels consisted of *n*-heptane, isooctane, toluene, ethanol and diisobutylene and fuel sensitivities (RON-MON) in the fuel blends ranged from two to nine. The operating conditions for the engine were $p_{\text{in}} = 0.1$ and 0.2 MPa, $T_{\text{in}} = 80$ and 250 °C, $\phi = 0.25$ in air and engine speed 1200 rpm. A semidetailed chemical kinetic model (142 species and 672 reactions) for gasoline surrogate fuels, validated against ignition data from experiments conducted in shock tubes for gasoline surrogate fuel blends at $1.0 \leq p \leq 5.0$ MPa, $700 \leq T \leq 1200$ K and $\phi = 1.0$, was successfully used to qualitatively predict the HCCI experiments using a single zone modelling approach. The fuel blends that had higher fuel sensitivity were more resistant to autoignition for low intake temperature and high intake pressure and less resistant to autoignition for high intake temperature and low intake pressure. A sensitivity analysis shows that at high intake temperature the chemistry of the fuels ethanol, toluene and diisobutylene helps to advance ignition. This is consistent with the trend that fuels with the least negative temperature coefficient (NTC) behaviour show the highest octane sensitivity, and become less resistant to autoignition at high intake temperatures. For high intake pressure the sensitivity analysis shows that fuels in the fuel blend with no NTC behaviour consume OH radicals and acts as a radical scavenger for the fuels with NTC behaviour. This is consistent with the observed trend of an increase in RON and fuel sensitivity. With data from shock tube experiments in the literature and HCCI modelling in this work, a correlation between the reciprocal pressure exponent on the ignition delay to the fuel sensitivity and volume percentage of single-stage ignition fuel in the fuel blend was found. Higher fuel sensitivity and single-stage fuel content generally gives a lower value of the pressure exponent. This helps to explain the results obtained while boosting the intake pressure in the HCCI engine.

10/00208 Heat transfer from a turbulent swirling inverse diffusion flame to a flat surface

Zhen, H. S. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2740–2748.

The heat transfer characteristics of a turbulent and swirling inverse diffusion flame (IDF) impinging vertically normal to a flat surface were investigated experimentally. The heat flux was measured by a heat flux sensor, Vatell HFM-6D/H. The effects of Reynolds number, overall equivalence ratio, nozzle-to-surface distance H and swirl number on the heat flux distributions were examined. The comparison of heat transfer of impinging IDFs with and without swirl was also conducted. The experimental results showed that the swirling effect influences the local heat flux in three ways. (1) The heat transfer at the stagnation point is severely suppressed. (2) The peak of local heat flux dwells at a radial distance from the stagnation point. (3) The radial position of peak local heat flux shifts farther away from the stagnation point with increasing H. There exists an optimum value of H at which the heat transfer to the target surface is the maximum and the optimum H increases with increasing ϕ while the Reynolds number and the swirl number are unchanged. The comparison of IDFs revealed that the swirling IDF has more complete combustion and thus it is accompanied by higher heat transfer rates at small H at which there exists a cool core in the case of the non-swirling IDF. The IDF, however, has worse heat transfer at higher H where the non-swirling IDF achieves complete combustion while the swirling IDF has been cooled by the entrained ambient air. Upon comparing the swirling and non-swirling IDFs at the same Re and ϕ, their respective optimum H showed an unfavorable effect of swirl on the overall heat transfer rate which has a reduction of up to 25% in the swirling IDF compared with the non-swirling IDF.

10/00209 Identification of intermediates in an *n*-heptane/oxygen/argon low-pressure premixed laminar flame using synchrotron radiation

Yao, C. *et al. Fuel*, 2009, 88, (9), 1752–1757.

This study was performed with the use of tunable vacuum ultraviolet lasers for molecular beam sampling mass spectrometry to detect the intermediates of a premixed *n*-heptane/oxygen/argon laminar low-pressure flame. In this experiment, 24 intermediate species were identified and quantified by the photoionization mass and efficiency spectra at a stoichiometric mixture of *n*-heptane/oxygen highly diluted by argon gas. The mole fraction profiles of these species at different flame positions are presented. The results show that the main intermediates are ketone and ether in the initial combustion period and these species then further oxidize to hydrocarbons. Of all the species, the concentrations of ethylene and polycyclic aromatic hydrocarbons are the highest concentration up to 10^{-2} and the lowest concentration to 10^{-5} in the mole fraction, respectively, at selective flame position. In addition, alkine like propyne exhibits very similar mole fraction profiles with that of benzene in the *n*-heptane flame. The results provide the strong evidence that benzene production correlates to alkine production in the flame and reinforces, at least qualitatively, the role of propyne species in the benzene formation mechanism. Finally, the distribution of 24 typical species in the flame is correlated with temperature, which is important in establishing the oxidation mechanism of hydrocarbon fuels.

10/00210 Jevons' Paradox revisited: the evidence for backfire from improved energy efficiency

Sorrell, S. *Energy Policy*, 2009, 37, (4), 1456–1469.

Beginning with William Stanley Jevons in 1865, a number of authors have claimed that economically justified energy-efficiency improvements will increase rather than reduce energy consumption. 'Jevons Paradox' is extremely difficult to test empirically, but could have profound implications for energy and climate policy. This paper summarizes and critiques the arguments and evidence that have been cited in support of Jevons' Paradox, focusing in particular on the work of Len Brookes and Harry Saunders. It identifies some empirical and theoretical weaknesses in these arguments, highlights the questions they raise for economic orthodoxy and points to some interesting parallels between these arguments and those used by the 'biophysical' school of ecological economics. While the evidence in favour of 'Jevons Paradox' is far from conclusive, it does suggest that economy-wide rebound effects are larger than is conventionally assumed and that energy plays a more important role in driving productivity improvements and economic growth than is conventionally assumed.

10/00211 Kinetic studies of overlapping pyrolysis reactions in industrial waste activated sludge

Yang, X. *et al. Bioresource Technology*, 2009, 100, (14), 3663–3668.

A sludge pyrolytic kinetics model was established in this study. Two types of sewage sludge from different industrial wastewater treatment plant produced different derivative thermogravimetry (DTG) shapes with an overlapping pattern. The multi-heating rate method was conducted to evaluate the kinetics for obtaining reasonable pyrolysis mechanisms and DTG curves were divided into several peaks using the Lorentz fitting method based on the composition of the sludge and the desire for precision. The peaks formed corresponded to the pyrolysis reactions of volatile matter, microbe cells, proteins, inorganic substances and char respectively, which can be reasonably explained based on the results from the flue gas analyser and the chemical analysis. Two types of sewage sludge were found to have similar pyrolysis mechanisms. Reasonable reasons were also given to explain the distortion and lag observed in the DTG curves and pyrolysis mechanism.

10/00212 Laser-induced radical generation and evolution to a self-sustaining flame

Beduneau, J. L. *et al. Combustion and Flame*, 2009, 156, (3), 642–656.

Images and emission spectra of sparks produced by laser-induced breakdown of methane and propane air mixtures were investigated with a high degree of spatial and temporal resolution. The laser-induced breakdown was generated by focusing a 532-nm nanosecond pulse from a Q-switched Nd:YAG laser. The data were collected using an intensified high-speed camera and a single/multi-fibre Cassegrain optics system coupled to an ICCD spectrometer. Emission spectra of OH*, CN*, CH*, and C_2* radicals were also collected using spectra boxes. The results provided information about the different stages of the laser-induced breakdown, with a specific focus on the transition from a flame kernel to a self-sustaining flame. The plasma shape and emission spectrum were reproducible. The differences in the size of the flame kernel and the evolution of the radical emissions were analysed for mixtures that fired or misfired. The impact of the level of radicals in the flame kernel was a critical parameter for the firing process, starting around 1 μs after the laser-induced breakdown. The transition from plasma cooling to the classical chemical reactions in the combustion zone was analysed. Even though the flame kernel size was directly linked to the spark energy, this was not a key parameter toward evolution to a self-sustaining flame. The Taylor blast wave theory was used to plot the location of the shock based on the evolution of the flame kernel size. The location was calculated using a laser-supported detonation model. A very good correlation was observed with the hot gas ignition process. The results provided information about the process leading to firing or misfiring for similar environments, resulting in a better understanding of the laser breakdown phenomena and the means of utilizing this technique in an industrial context.

10/00213 Nitrogen dilution effect on the flammability limits for hydrocarbons

Chen, C.-C. *et al. Journal of Hazardous Materials*, 2009, 166, (2–3), 880–890.

Theoretical models to predict the upper/lower flammability limits of hydrocarbons diluted with inert nitrogen gas are proposed in this study. It is found that there are linear relations between the reciprocal of the upper/lower flammability limits and the reciprocal of the molar fraction of hydrocarbon in the hydrocarbon/inert nitrogen mixture. Such linearity is examined by experimental data reported in the literature, which include the cases of methane, propane, ethylene and propylene. The R-squared values (R^2) of the regression lines of the cases explored are all greater than 0.989 for upper flammability limit (UFL). The theoretical slope of the predictive line for lower flammability limit (LFL) is found to be very close to zero for all explored cases; and this result successfully explains the experimental fact that adding inert nitrogen to a flammable material has very limited effect on LFL. Because limit oxygen concentration (LOC) could be taken as the intersectional point of the UFL curve and LFL curve, a LOC-based method is proposed to predict the slope of the UFL curve when experimental data of UFL are not available. This LOC-based method predicts the UFL with average error ranging from 2.17% to 5.84% and maximum error ranging from 8.58% to 12.18% for the cases explored. The predictive models for inert gas of nitrogen are also extended to the case of inert gas other than nitrogen. Through the extended models, it was found that the inert ability of an inert gas depends on its mean molar heat capacity at the adiabatic flame temperature. Theoretical calculation shows that the inert abilities of carbon dioxide, steam, nitrogen and helium are in the following order: carbon dioxide > steam > nitrogen > helium; and this sequence conforms to the existing experimental data reported in the literature.

10/00214 Numerical prediction on the erosion in the hearth of a blast furnace during tapping proces

Chang, C. M. *et al. International Communications in Heat and Mass Transfer*, 2009, 36, (5), 480–490.

The erosion caused by mass transfer in hearth is the most important factor for determining blast furnace campaign life. To support a helpful insight information of mass transfer for the hearth of the No. 2 blast furnace at CSC (China Steel Corporation), a numerical model including the mass transfer of carbon in thermal convective flow from a blast furnace hearth has been developed during the steady tapping process (based on a uninterrupted tapping process assumption). The three-dimensional Navier–Stokes equation combined with the transport equations of energy and species with conjugate heat transfer and physical dissolution source is solved by the finite control volume scheme subjected to the segregated iterate under propriety boundary conditions. The results showed the concentration distribution of carbon expressed in terms of mass flux for analysing the erosion of carbon brick in the blast furnace hearth with the different conditions including the status of dead-man, production of liquid iron, carbon concentration at the inlet, and porosity distribution in coke zone during tapping process at steady state. The result is useful to mitigate the erosion caused by mass transfer, and prolong the life span of the blast furnace.

10/00215 Numerical prediction on the variation of temperature in the eroded blast furnace hearth with titanium dioxide in hot metal

Lin, C. H. *et al. International Communications in Heat and Mass Transfer*, 2009, 36, (4), 335–341.

This paper numerically predicts the decrease in temperature of the eroded hearth of the blast furnace with floating deadman (coke zone) case for Port Kembla no. 5 blast furnace (PKBF5) by solving the Navier–Stokes equation, the thermal-energy-balance equation with conjugated heat transfer, and the mass transfer equation with the effect of chemical reaction during tapping process at steady state. The chemical reaction is generated by titanium dioxide (TiO_2) reacting with saturated carbon in hot metal. The following calculations are done by using a commercial computational fluid dynamics (CFD) package, FLUENT (version 6.2), with a segregated model. As shown in the results, on the basis of the flow pattern of liquid iron, the inlet selection of adding TiO_2 may be far away from the taphole. The calculated temperature variation in the damaged hearth by reaction is significant, but that on the other side of the hearth without adding TiO_2 isn't influenced. Additionally, the numerical temperature data of different locations may be examined by the blast furnace operators to judge the effect of lowering temperature.

10/00216 Numerical simulation of chemical looping combustion process with $CaSO_4$ oxygen carrier

Deng, Z. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (4), 368–375.

Chemical-looping combustion (CLC) is a promising technology for the combustion of gas or solid fuel with efficient use of energy and inherent separation of CO_2. The technique involves the use of an oxygen carrier which transfers oxygen from combustion air to the fuel, and hence a direct contact between air and fuel is avoided. A chemical-looping combustion system consists of a fuel reactor and an air reactor. A metal oxide is used as oxygen carrier that circulates between the two reactors. The air reactor is a high velocity fluidized bed where the oxygen carrier particles are transported together with the air stream to the top of the air reactor, where they are then transferred to the fuel reactor using a cyclone. The fuel reactor is a bubbling fluidized bed reactor where oxygen carrier particles react with hydrocarbon fuel and get reduced. The reduced oxygen carrier particles are transported back to the air reactor where they react with oxygen in the air and are oxidized back to metal oxide. The exhaust from the fuel reactor mainly consists of CO_2 and water vapour. After condensation of the water in the exit gas from the fuel reactor, the remaining CO_2 gas is compressed and cooled to yield liquid CO_2, which can be disposed of in various ways. In this work, the reaction kinetics model of the fuel reactor ($CaSO_4 + H_2$) was developed by means of the commercial code FLUENT. The bubble formation and the relation between bubble formation and molar fraction of products in gas phase were well captured by CFD simulation. Computational results from the simulation also showed low fuel conversion rate. The conversion of H_2 was about 34% partially due to fast, large bubbles rising through the reactor, low bed temperature and large particles diameter.

10/00217 Pyrolysis kinetics of olive residue/plastic mixtures by non-isothermal thermogravimetry

Aboulkas, A. *et al. Fuel Processing Technology*, 2009, 90, (5), 722–728.

TGA studies of a pyrolytic decomposition of mixtures of olive residue/plastic were carried out. The investigation was made at temperatures ranging from 300 to 1273 K) in a nitrogen atmosphere at four heating rates $\beta = 2$, 10, 20 and 50 K min^{-1}. High density polyethylene (HDPE), low density polyethylene (LDPE), polypropylene (PP) and polystyrene (PS) were selected as plastic samples. Based on the results obtained, three thermal stages were identified during the thermal degradation. The first two were dominated by the olive residue pyrolysis, while the third was linked to the plastics pyrolysis, which occurred at much higher temperatures. Discrepancies between the experimental and calculated TG/DTG profiles were considered as a measurement of the extent of interactions occurring on pyrolysis olive residue/plastic mixtures. The maximum degradation temperatures of each component in the mixture were higher than those of the individual components. These experimental results indicate a significant synergistic effect during olive residue and plastic co-pyrolysis at the high temperature region. In addition, a kinetic analysis was performed to fit thermogravimetric data. A reasonable fit to the experimental data was obtained for all materials and their mixtures.

10/00218 Rapid and catalytic pyrolysis of corn stalks

Uzun, B. B. and Sarioğlu, N. *Fuel Processing Technology*, 2009, 90, (5), 705–716.

Non-catalytic and catalytic rapid pyrolysis of corn stalks was studied in a tubular fixed-bed reactor. The optimum operating conditions giving the highest liquid yield was determined as pyrolysis temperature of 500 °C, sweeping gas flow rate of 400 $cm^3 min^{-1}$ and heating rate of 500 °C min^{-1}. In the catalytic process, rapid pyrolysis of stalks was performed at the optimum conditions with catalysts such as ZSM-5, HY and USY. The highest liquid yield from the catalytic pyrolysis was 27.55% with ZSM-5, while the oil from non-catalytic pyrolysis was 33.30%. In the last part, various spectroscopic and chromatographic methods were applied for characterization of bio-oils. Although catalytic pyrolysis converts the long chains of alkanes and alkenes of the oils into lower weight hydrocarbons, the obtained oil yields were lower than those of non-catalytic pyrolysis. USY catalyst gives the highest amount of aromatics among the catalysts used. Moreover, TG–DTA analyses were applied on raw materials to investigate thermal degradation of corn stalks and calculate the kinetic parameters.

10/00219 Reconstruction of soot temperature and volume fraction profiles of an asymmetric flame using stereoscopic tomography

Huang, Q. *et al. Combustion and Flame*, 2009, 156, (3), 565–573.

The present study attempts to reconstruct soot temperature and volume fraction distributions for the asymmetric diffusive flame using a tomography technique. A high-resolution camera equipped with a stereo adapter was employed to capture stereoscopic flame images, which were used to obtain monochromatic line-of-sight flame emission projections within the visible range. A matrix-decomposition-based least squares algorithm was introduced to reconstruct the emission intensity distributions in the flame sections. The retrieved intensities were used to infer local soot temperature and volume fraction. Numerical assessments show that for soot volume fraction measurement, the system signal-to-noise ratio should be larger than 62.5 dB. The proposed tomography system was found to be capable of symmetric and asymmetric flame measurements.

10/00220 Residence time investigation of a multiple hearth kiln using mineral tracers

Thomas, R. *et al. Chemical Engineering and Processing: Process Intensification*, 2009, 48, (4), 950–954.

Kaolin is used in many applications (e.g. paint, plastic and rubber) due to its unique properties, including fine particle size, brightness and chemical inertness. Properties can be improved by calcination, heating the kaolin to high temperatures inducing physico-chemical transformations. If calcination time is excessive, kaolin becomes harder and abrasive, due to mullite formation. This is detrimental to product quality; causing processing problems and machinery damage. If calcination time is too short, the kaolin is not fully calcined, becoming highly reactive, an issue for pharmaceutical applications. By controlling the exposure time to high temperature, such negative effects are minimized. Multiple hearth calciners are often used for this transformation, but their operating conditions and configuration make it difficult to determine kaolin residence time. To improve product consistency, trials were performed to measure the residence time distribution of an industrial furnace used to calcine kaolin. Titania, TiO_2, and talc, $Mg_3Si_4O_{10}(OH)_2$, were used to individually dope the kaolin, $Al_2Si_2O_5(OH)_4$, and the concentration of these mineral tracers was detected using X-ray fluorescence. Talc was the preferred mineral tracer, with a mean residence time of 42 min under standard operating conditions, with a throughput of 5.3 tonnes h^{-1} of 0 wt% moisture feed.

10/00221 Study on premixed combustion in cylindrical micro combustors: transient flame behavior and wall heat flux

Li, J. *et al. Experimental Thermal and Fluid Science*, 2009, 33, (4), 764–773.

The micro combustor is a key component of the micro thermophotovoltaic (TPV) system. Improving the wall temperature of the micro combustor is an effective way to elevate the system efficiency. An experimental study on the wall temperature and radiation heat flux of a series of cylindrical micro combustors (with a backward-facing step) was carried out. For the micro combustors with $d = 2$ mm, the regime of successful ignition (under the cold wall condition) was identified for different combustor lengths. Acoustic emission was detected for some cases and the emitted sound was recorded and analysed. Under the steady-state condition, the effects of the combustor diameter (d), combustor length (L), flow velocity (u_0) and fuel–air equivalence ratio (Φ) on the wall temperature distribution were investigated by measuring the detailed wall temperature profiles. In the case that the micro combustor is working as an emitter, the optimum efficiency was found at $\Phi \approx 0.8$, independent of the combustor dimensions (d and L) and the flow velocity. Under the experimental conditions employed in the present study, the positions of the peak wall temperature were found to be about 8–11 mm and 4–6 mm from the step for the $d = 3$ mm and $d = 2$ mm micro combustors, respectively, which are 8–11 and 8–12 times of their respective step heights. This result suggests that the backward-facing step employed in the combustor design is effective in stabilizing the flame position.

10/00222 Thermogravimetric study of interactions in the pyrolysis of blends of coal with radiata pine sawdust

Ulloa, C. A. *et al. Fuel Processing Technology*, 2009, 90, (4), 583–590.

The co-pyrolysis of coal-biomass blends were studied by using thermogravimetric analysis to look for thermal events indicating interactions that could cause synergic or inhibitory effects during the first stage in the co-combustion of these materials. Two coals from different rank were selected for the study and combined with radiata pine sawdust, the selected biomass compound. Pyrolysis assays were carried out on the individual components and the binary coal-sawdust blends (50% p/p) at different heating rates (10, 30, 50 °C/min) until reaching a maximum temperature of 1200 °C. The individual components behaved as expected and as is widely described in the specialized literature. Interactions detected in the blends resulted in greater-than-expected volatile yield values. These interactions were produced at pyrolysis temperatures over 400 °C, when most of the components in the blend are devolatilized, and are attributed to secondary reactions that inhibit the formation of char.

Fire safety

10/00223 An inter-comparison exercise on CFD model capabilities to predict a hydrogen explosion in a simulated vehicle refuelling environment

Makarov, D. *et al. International Journal of Hydrogen Energy*, 2009, 34, (6), 2800–2814.

The paper describes the comparison of simulations of a hydrogen explosion experiment in an environment simulating a vehicle refuelling station. The exercise was performed in 2007 within the European Commission-funded Network of Excellence 'Hydrogen Safety as an Energy Carrier' (http://www.hysafe.org), which facilitates the safe introduction of hydrogen technologies and infrastructure. The experiment in a mock-up of a hydrogen refuelling station was conducted jointly by Shell Global Solutions (UK) and the Health and Safety Laboratory (UK) in order to study the potential hazards and consequences associated with a hydrogen–air mixture explosion. The 'worst-case' scenario of a stoichiometric hydrogen–air mixture explosion was offered to the network partners for this simulation exercise. Simulations were conducted by a total of seven partners using different models and numerical codes with the intention of predicting/reproducing pressure dynamics in different locations and of evaluating the performance of different combustion codes and models in realistic large-scale conditions. The paper briefly details the models and numerical codes used, and presents the simulated pressure transients obtained by the partners in comparison with the experimental pressure records. The comparative model analysis was made based on achieved simulation results, where the simulated maximum overpressure and the characteristic rate of pressure rise were treated as major output parameters. A contribution to hydrogen safety was made in the form of a description of the models, their performance and an analysis of the results for their cross-fertilization where possible.

10/00224 Detailed simulations of the transient hydrogen mixing, leakage and flammability in air in simple geometries

Vudumu, S. K. and Koylu, U. O. *International Journal of Hydrogen Energy*, 2009, 34, (6), 2824–2833.

During an accidental release, hydrogen disperses very quickly in air due to a relatively high density difference. A comprehensive understanding of the transient behaviour of hydrogen mixing and the associated flammability limits in air is essential to support the fire safety and prevention guidelines. In this study, a buoyancy diffusion computational model is developed to simultaneously solve for the complete set of equations governing the unsteady flow of hydrogen. A simple vertical cylinder is considered to investigate the transient behaviour of hydrogen mixing, especially at relatively short times, for different release scenarios: (i) the sudden release of hydrogen at the cylinder bottom into air with open, partially open, and closed tops, and (ii) small hydrogen jet leaks at the bottom into a closed geometry. Other cases involving the hydrogen releases/leaks at the cylinder top are also explored to quantify the relative roles of buoyancy and diffusion in the mixing process. The numerical simulations display the spatial and temporal distributions of hydrogen for all the configurations studied. The complex flow patterns demonstrate the fast formation of flammable zones with implications in the safe and efficient use of hydrogen in various applications.

10/00225 Development of probabilistic models to estimate fire-induced cable damage at nuclear power plants

Valbuena, G. and Modarres, M. *Nuclear Engineering and Design*, 2009, 239, (6), 1113–1127.

Numerous probabilistic risk assessments (PRAs) have shown that fire is a major contributor to nuclear power plant (NPP) risks. However, prediction and estimation of the likelihood of fire-induced damage to electrical cables and circuits and their potential effects on the safety of the NPPs are still a practical challenge, particularly because of the lack of physics-based models with which to perform consistent and objective assessments. This paper contains a discussion of two models – the heat transfer and the IR 'K-factor' models – to estimate the likelihood of fire-induced cable damage given a specified fire profile. The results of this research will help to (1) develop a consistent framework to estimate the likelihood of fire-induced cable failure modes, and (2) develop some guidance to evaluate and/or reduce the risks associated with these failure modes in existing and new NPPs. The models are developed (i.e. their parameters are estimated) based on the test data from various fire damage tests sponsored by the nuclear industry and the US Nuclear Regulatory Commission (NRC). Among the models evaluated, the physics-based heat transfer model is promising because it takes into account the properties and characteristics of the cables and cable materials and the characteristics of the thermal insult. This model can be used to estimate the probability of cable damage (P_{CD}) under different thermal conditions.

10/00226 Laminar burning velocity and Markstein length of nitrogen diluted natural gas/hydrogen/air mixtures at normal, reduced and elevated pressures

Miao, H. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 3145–3155.

Flame propagation of premixed nitrogen diluted natural gas/hydrogen/air mixtures was studied in a constant volume combustion bomb under various initial pressures. Laminar burning velocities and Markstein lengths were obtained for the diluted stoichiometric fuel/air mixtures with different hydrogen fractions and diluent ratios under various initial pressures. The results showed that both unstretched flame speed and unstretched burning velocity are reduced with the increase in initial pressure (except when the hydrogen fraction is 80%) as well as diluent ratio. The velocity reduction rate due to diluent addition is determined mainly by hydrogen fraction and diluent ratio, and the effect of initial pressure is negligible. Flame stability was studied by analysing Markstein length. It was found that the increase of initial pressure and hydrogen fraction decreases flame stability and the flame tends to be more stable with the addition of diluent gas. Generally speaking, Markstein length of a fuel with low hydrogen fraction is more sensitive to the change of initial pressure than that of a one with high hydrogen fraction.

10/00227 Simulation of airflow in one- and two-room enclosures containing a fire source

Stavrakakis, G. M. and Markatos, N. C. *International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2690–2703.

In this study, the airflow in a room that contains a heat source is simulated numerically. The flow is considered turbulent and buoyant. The results of the mathematical model are validated with available experimental data at specific locations in the domain. A simple geometry is adopted, consisting of a room with a door that plays the role of both inlet–outlet for the fluid (air). At the centre of the room a methane burner is placed to serve as a heat source. The problem is simulated using two turbulence models, the well-known standard k–ϵ model and the RNG k–ϵ model, both modified to account for buoyancy effects on turbulence. The burner is considered as a volumetric heat source. It is concluded that the fire plume development as well as the distributions of velocity and temperature are reasonably well predicted. Following this conclusion, both models are also applied to a different, more complex geometry that consisted of two rooms communicating via a door, while the heat source was placed in the first room. Unfortunately, there are no experimental data to compare with for this case, but the results appear plausible. Finally, important design factors, such as mass flow rates and neutral-plane heights, are calculated utilizing the CFD results, and are compared with those obtained by well-known empirical correlations. It is concluded that the bi-directional flow existing through the burning-room vent is similarly predicted by both turbulence models; the RNG k–ϵ model leading to higher, and more accurate predictions of temperature variations within the hot upper layer, at least for the single-room case.

09 PROCESS HEATING, POWER AND INCINERATION

Energy applications in industry

10/00228 Numerical modelling of axial bed-to-wall heat transfer in a circulating fluidized bed combustor

Gnanapragasam, N. V. and Reddy, B. V. *International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1657–1666.

The water-wall surfaces located above the secondary air inlet within the circulating fluidized bed (CFB) combustor are exposed to the axial bed-to-wall heat transfer process. The axial bed-to-wall heat transfer coefficients are estimated for three different axial voidage profiles (covering three widely occurring average particle concentrations) in order to investigate the effect of voidage, time, initial and fixed temperature of the bed and annulus, and gas gap between wall and solid particles; on the axial heat transfer process. A 2D thermal energy balance model is developed to estimate the axial heat transfer values for the gas–solid suspension along the height of the riser column with horizontally changing mass distribution. The gas–solid mass distribution is fixed with time thus providing a spectrum of changes in axial bed-to-wall heat transfer profile with time. The current work provides an opportunity to understand the axial heat transfer relationship with particle concentration and instantaneous behaviour. The results from the work show that: (i) first few seconds of the suspension temperature near the wall has maximum energy thus providing a small time frame to transfer more heat to the surface (CFB wall); (ii) both axial and horizontal particle concentrations (influenced by the operating conditions) affect the axial heat transfer locally; (iii) initial temperature of the bed between average and maximum values provide end limits for the axial heat transfer; (iv) annulus region has higher thermal energy than the core due to increased particle presence; and (v) a particle-free zone near the wall (gas gap) having a maximum thickness of 1 mm, tends to reduce up to 25% of axial heat transfer value. The model trends have close agreement with experimental trends from published literature; but the model values differ when correlating with real values due to inconsistencies in riser diameter and nature of variation in parameters.

10/00229 3D hybrid Cartesian/immersed-boundary finite-element analysis of heat and flow patterns in a two-roll mill

Chiu, C. L. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1677–1689.

A fully three-dimensional time-dependent Navier–Stokes model with forced convection is developed to numerically investigate the heat and flow patterns of the two-roll mill system with two inner rotating cylinders. Such direct numerical simulations are usually limited by the difficulties from huge computational cost and complex boundary treatment. For a fast numerical process, the operator-splitting scheme can be used with the balanced tensor diffusivity (BTD) term to advance the solution in temporal evolution. To implement the calculation over a Cartesian grid, the hybrid Cartesian/immersed-boundary finite-element method is employed for spatial discretization. In the authors' previous study, a simplified two-dimensional numerical model was developed to analyse the heat and flow patterns on the cross section of two-roll-mill flow under the assumption of infinite length in the third (vertical) direction. However, the two-dimensional solutions could not completely represent the realistic physical phenomena unless a three-dimensional algorithm is developed. In this study, particular attention was paid to develop a three-dimensional model to investigate the vertical heat and flow behaviours, including three-dimensional features of the vortex structure, periodic oscillation and chaotic instabilities. It is found that the proposed three-dimensional model is able to cover the two-dimensional features if the assumptions of two-dimensional conditions are fulfilled.

10/00230 A qualitative reliability and operability analysis of an integrated reforming combined cycle plant with CO_2 capture

Nord, L. O. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (4), 411–421.

Most of the current carbon dioxide capture technologies are associated with large energy penalties that reduce their economic viability. Efficiency has therefore become the most important issue when designing and selecting power plants with carbon dioxide capture. Other aspects, like reliability and operability, have been given less importance, if any at all, in the literature. This article deals with qualitative reliability and operability analyses of an integrated reforming combined cycle concept. The plant reforms natural gas into a syngas, the carbon is separated out as carbon dioxide after a water-gas shift section, and the hydrogen-rich fuel is used for a gas turbine. The qualitative reliability analysis in the article consists of a functional analysis followed by a failure mode, effects, and criticality analysis (FMECA). The operability analysis introduces the comparative complexity indicator (CCI) concept. Functional analysis and FMECA are important steps in a system reliability analysis, as they can serve as a platform and basis for further analysis. Also, the results from the FMECA can be interesting for determining how the failures propagate through the system and their effects on the operation of the process. The CCI is a helpful tool in choosing the level of integration and to investigate whether or not to include a certain process feature. Incorporating the analytical approach presented in the article during the design stage of a plant can be advantageous for the overall plant performance.

10/00231 Complex chemical systems with power production driven by heat and mass transfer

Sieniutycz, S. *International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2453–2465.

This investigates power production in complex multireaction systems propelled by either uncoupled or coupled multicomponent mass transfer. The considered system contains two mass reservoirs, one supplying and one taking out the species, and a power-producing reactor undergoing the chemical transformations characterized by multiple (vector) efficiencies. To establish a suitable basis for these efficiencies, an approach is applied that implements balances of molar flows and reaction invariants to complex chemical systems with power production. Reaction invariants, i.e. quantities that take the same values during a reaction, follow by linear transformations of molar flows of the species. Flux balances for the reacting mixture may be written down by equating these reaction invariants before and after the reactor. Obtained efficiency formulas are applied for steady-state chemical machines working at the maximum production of power. Total output of produced power is maximized at constraints which take into account the (coupled or uncoupled) mass transport and efficiency of power generation. Special attention is given to non-isothermal power systems, stoichiometric mixtures and internal dissipation within the chemical reactor. Optimization models lead to optimal functions that describe thermokinetic limits on power production or consumption and extend reversible chemical work W_{rev} to situations in which reduction of chemical efficiencies, caused by finite rates, is essential. The classical thermostatic theory of reversible work is recovered from the present thermokinetic theory in the case of quasistatic rates and vanishing dissipation.

10/00232 Effect of a draft tube on gas–liquid jet boundaries in a gas–solid fluidized bed

Briens, C. *et al. Chemical Engineering and Processing: Process Intensification*, 2009, 48, (4), 871–877.

Liquids are injected into fluidized beds in a variety of industrial processes. Installing a draft tube downstream of the nozzle works to optimize the jet–bed interactions so that the liquid feed is more evenly dispersed amongst the bed solids. Triboelectric probes were used to confirm the location of the 'mixing zone' inside the draft tube, and also to study the effects a draft tube had on the upstream and downstream jet boundaries. This shows how the presence of a draft tube affects the expansion angle and the penetration depth of a gas–liquid jet in a fluidized bed.

10/00233 Experimental observations on the different mechanisms for solid ejection in gas-fluidized beds

Almendros-Ibáñez, J. A. *et al. Chemical Engineering and Processing: Process Intensification*, 2009, 48, (3), 734–744.

This work presents an experimental study of the ejection velocity for different mechanisms of solid ejection in fluidized beds. The experiments were carried out in a 2D fluidized bed, where the bubble eruptions were recorded with a frequency of 250 frames per second using a high speed video camera with a resolution of 1.3 megapixels. The results show that in isolated bubble eruption, the dome velocity is significantly reduced by the effect of a group of raining particles in the form of stalactites within the bubble. Higher velocities are observed when bubble coalescence takes place. If bubbles coalesce before the leading bubble breaks, the momentum of the trailing bubble together with the increase in the throughflow accelerate the dome of the leading bubble. In contrast, when coalescence occurs after the breakage of the leading bubble, the wake of the trailing bubble is projected into the freeboard with a very high velocity (wake spike mechanism). The last observed mechanism, the jet spike mechanism, occurs when a stream of bubbles reaches the bed surface following the path opened by the previous bubbles. A cloud of particles moving upward is observed, although their velocities are not as high as in the wake spike mechanism due to the interchange of momentum during the collisions with other particles. Finally, an explanation for some of the patterns of gas release from erupting bubbles recently observed in another study is proposed.

10/00234 Fluid-particle mass transport of cupric chloride hydrolysis in a fluidized bed

Haseli, Y. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2507–2515.

This paper examines the mass transport phenomena of a hydrolysis reaction involving cupric chloride particles and superheated steam in a fluidized bed, as a part of the copper–chlorine thermochemical cycle for nuclear-based hydrogen production. The Gómez-Barea method was extended and utilized for the purpose of this study. A uniform reaction model (volumetric model) and shrinking core model were used for limiting cases of the conversion processes. Using the solution procedures developed for each case, the effects of different parameters (such as the superficial gas velocity, bed inventory, and process temperature) were investigated in terms of the conversion of $CuCl_2$ particles and steam.

10/00235 Fully developed thermal behaviors for parallel flow microchannel heat exchanger

Al-Nimr, M. A. *et al. International Communications in Heat and Mass Transfer*, 2009, 36, (4), 385–390.

The hydrodynamics and thermal behaviours of the flow in micro-heat exchanger parallel-plate are investigated numerically. The model that combines both the continuum approach and the possibility of slip at the boundary is adopted in the study. Effects of different parameters, such as, Knudsen number (*Kn*), heat capacity ratio (Cr), the effectiveness (*e*) and number of transfer units (NTU) are investigated. It is found that both the velocity slip and the temperature jump at the walls increase with increasing *Kn*. On the other hand, at low values of *Kn*, the NTU increases with increasing Cr, but at high values of *Kn* the NTU decreases with increasing Cr. With regard to the effect of Cr on *e*, it is found that increasing Cr leads to a reduction in *e* and for all *Kn*.

10/00236 Heat transfer enhancement and pressure drop characteristics of TiO_2–water nanofluid in a double-tube counter flow heat exchanger

Duangthongsuk, W. and Wongwises, S. *International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 2059–2067.

This article reports an experimental study on the forced convective heat transfer and flow characteristics of a nanofluid consisting of water and 0.2 vol.% TiO_2 nanoparticles. The heat transfer coefficient and friction factor of the TiO_2–water nanofluid flowing in a horizontal double-tube counter flow heat exchanger under turbulent flow conditions are investigated. The Degussa P25 TiO_2 nanoparticles of about 21 nm diameter are used in the present study. The results show that the convective heat transfer coefficient of nanofluid is slightly higher than that of the base liquid by about 6–11%. The heat transfer coefficient of the nanofluid increases with an increase in the mass flow rate of the hot water and nanofluid, and increases with a decrease in the nanofluid temperature, and the temperature of the heating fluid has no significant effect on the heat transfer coefficient of the nanofluid. It is also seen that the Gnielinski equation failed to predict the heat transfer coefficient of the nanofluid. Finally, the use of the nanofluid has a little penalty in pressure drop.

10/00237 Impact of operating conditions on the performance of the external loop in a CFB reactor

Yang, S. *et al. Chemical Engineering and Processing: Process Intensification*, 2009, 48, (4), 921–926.

The effects of operating parameters such as fluidizing gas velocity U_g and total solid inventory M_t on the performance of the external loop composed by the loop seal and standpipe in a circulating fluidized bed (CFB) system were often ignored in the existing studies and the limited data are still in controversy. In this paper, the characteristics of gas–solid flow in the external loop was studied in a CFB cold test rig with a square riser of $0.1\,m \times 0.1\,m$ in cross-section and 3.2 m in height. The results show that solid circulating rate G_s in the external loop is a function of the operating parameters such as M_t, U_g and aeration rate. An empirical equation was proposed for the G_s in the external loop with the operating parameters in the riser. The pressure drop across the loop seal is directly proportional to G_s while is inversely proportional to the aeration rate. The pressure drop gradient, voidage and solid height in the standpipe are also influenced by the operating conditions. The controversy among the published literature was discussed and clarified. The results of present study indicated that the external loop cannot be isolated from the entire CFB system for quantitative performance evaluation.

10/00238 Modelling of the behavior of power electronic equipment to grid ripple control signal

Yang, Y. and Dennetière, S. *Electric Power Systems Research*, 2009, 79, (3), 443–448.

The paper presents time-domain simulation for power electronic device equivalent impedance computation at ripple control signal frequency. The ripple control used by the grid is a low frequency voltage signal superimposed at MV substation. In France, the frequency used by grid ripple control systems is 175 Hz. It is well known that some customer loads can disturb ripple control signal transmission such as capacitor bank, distributed generator, etc. These equipments can influence or disturb ripple control signal in two main ways: presence of a small impedance or an important interharmonic current injection at ripple control frequency. In transient state, even a symmetrical static converter can produce interharmonic currents. In site studies, some customer power electronic devices (variable speed drive for example) are often modelled by an infinite impedance at ripple control frequency. However, site measurements and simulations show that this simplification can cause in some case important error in ripple control signal level assessment. The main purpose of this study is to define ripple control frequency equivalent impedances of typical converters used in industry. The study shows that a voltage source converter (rectifier with dc capacitor structure) gives a relative small impedance at ripple control frequency. It is recommended to integrate this impedance in performing ripple control signal propagation study by means of frequency-domain software.

10/00239 Numerical study of heat exchanger effects on charge/discharge times of metal–hydrogen storage vessel

Mellouli, S. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 3005–3017.

In this paper a mathematical model has been developed to evaluate various designs of metal–hydrogen storage vessel (MHSV). This model which considers complex heat and mass transfer is numerically solved and a computer program is developed. The numerical results are compared to the measured data collected on three MHSV and a reasonable agreement is obtained. The performance of an MHSV is mainly denoted by the hydrogen storage time and the capacity of the absorption and desorption. Hence, a discussion based on these parameters has been done. Moreover, results concerning the impact of the heat exchanger configuration are given.

10/00240 Numerical study of the relationship between heat transfer enhancement and absolute vorticity flux along main flow direction in a channel formed by a flat tube bank fin with vortex generators

Chang, L.-M. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1794–1801.

The secondary flow is frequently used to enhance the convective heat transfer. In this paper, the cross-averaged absolute vorticity flux in the main flow direction is used to specify the intensity of the secondary flow produced by vortex generators that are mounted on a three-row flat tube bank fin surfaces. The relationship between the intensity of the secondary flow and the strength of convective heat transfer is studied using a numerical method. The results reveal that cross-averaged absolute vorticity flux in the main flow direction can reflect the intensity of the secondary flow; a significant relationship between this cross-averaged absolute vorticity flux and span-averaged Nusselt number exists for the case studied. This cross-averaged absolute vorticity flux can account only for the secondary flow effects on convective heat transfer but cannot quantify the effects of developing boundary layer on convective heat transfer.

10/00241 Performance analyses of VHTR plants with direct and indirect closed Brayton cycles and different working fluids

El-Genk, M. S. and Tournier, J.-M. *Progress in Nuclear Energy*, 2009, 51, (3), 556–572.

This paper investigated the performance of very high temperature reactor (VHTR) power plants with helium working fluid and direct and indirect Closed Brayton Cycles (CBCs), and with binary mixture working fluids of He–Xe and He–N_2 (molecular weight of 15 g/mole) and indirect CBCs. Also investigated are the effects of using low- and high-pressure compressors with intercooling, versus a single compressor, using bleed cooling the reactor pressure vessel in direct CBC helium plants, and varying the reactor exit temperature fr°m 700 °C to 950 °C on the plant thermal efficiency, cycle pressure ratio and the size of and number of stages in the turbine and compressor. Analyses are performed for a shaft rotation speed of 3000 rpm, reactor thermal power of 600 MW and a temperature pinch of 50 °C in the intermediate heat exchanger (IHX) for the indirect CBCs.

10/00242 Performance predictions of laminar and turbulent heat transfer and fluid flow of heat exchangers having large tube-diameter and large tube-row by artificial neural networks

Xie, G. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2484–2497.

In this work an artificial neural network (ANN) is used to correlate experimentally determined and numerically computed Nusselt numbers and friction factors of three kinds of fin-and-tube heat exchangers having plain fins, slit fins and fins with longitudinal delta-winglet vortex generators with large tube-diameter and large the number of tube rows. First the experimental data for training the network was picked up from the database of nine samples with tube outside diameter of 18 mm, number of tube rows of six, nine, 12, and Reynolds number between 4000 and 10,000. The artificial neural network configuration under consideration has 12 inputs of geometrical parameters and two outputs of heat transfer Nusselt number and fluid flow friction factor. The commonly implemented feed-forward back propagation algorithm was used to train the neural network and modify weights. Different networks with various numbers of hidden neurons and layers were assessed to find the best architecture for predicting heat transfer and flow friction. The deviation between the predictions and experimental data was less than 4%. Compared to correlations for prediction, the performance of the ANN-based prediction exhibits ANN superiority. Then the ANN training database was expanded to include experimental data and numerical data of other similar geometries by computational fluid dynamics (CFD) for turbulent and laminar cases with the Reynolds number of 1000–10,000. This in turn indicated the prediction has a good agreement with the combined database. The results suggest that the developed ANN model is generalized to predict the turbulent or/and laminar heat transfer and fluid flow of such three kinds of heat exchangers with large tube-diameter and large number of tube rows. Weights and biases corresponding to the neural network architecture are also provided. It is recommended that ANNs might be used to predict the performances of thermal systems in engineering applications, especially to model heat exchangers for heat transfer analysis.

10/00243 Separating group compositions in naphtha by adsorption and solvent extraction to improve olefin yields of steam cracking process

Liu, J.-C. *et al. Journal of Petroleum Science and Engineering*, 2009, 66, (3–4), 156–160.

In order to improve the steam cracking feeds, several model compounds including normal paraffins, iso-paraffins, cyclanes and aromatics were selected as the feeds of steam cracking process and the olefin yields were investigated. In the typical reaction conditions, the normal paraffins in the naphtha contribute most to the ethylene in the products; the iso-paraffins are the main sources of the propylene; the cyclanes mainly produce the butadiene and the aromatics can hardly produce olefins. According to this, the adsorption process and solvent extraction process were adopted to separate the group compositions in naphtha properly to optimize the cracking feeds. The n-paraffins in naphtha were gathered through adsorption process using 5A molecular sieves. The ethylene yield improved by 13% using the desorption oil rich in n-paraffins as the cracking feed. The aromatics and the cyclanes were extracted from the naphtha. Compared with the naphtha, the ethylene and propylene yields of the extraction raffinate oil were 3.0 and 1.5% higher respectively.

10/00244 The modelling of a hybrid combined cycle with pressurised fluidised bed combustion and CO_2 capture

Bryngelsson, M. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (3), 255–262.

This study investigates the possibility of capturing CO_2 from flue gas under pressurized conditions, which could prove to be beneficial in comparison to working under atmospheric conditions. Simulations of two hybrid combined cycles with pressurized fluidized bed combustion and CO_2 capture are presented. CO_2 is captured from pressurized flue gas by means of chemical absorption after the boiler but before expansion. The results show a CO_2 capture penalty of approximately 8 percentage points (including 90% CO_2 capture rate and compression to 110 bar), which makes the efficiency for the best performing cycle 43.9%. It is 5.2 percentage points higher than the most probable alternative, i.e. using a natural gas fired combined cycle and a pulverized coal fired condensing plant separately with the same fuel split ratio. The largest part of the penalty is associated with the lower mass flow of flue gas after CO_2 capture, which leads to a decrease in work output in the expander and potential for feed water heating. The penalty caused by the regeneration of absorbent is quite low, since the high pressure permits the use of potassium carbonate, which requires less regeneration heat than for example the more commonly proposed monoethanolamine. Although the efficiencies of the cycles look promising it will be important to perform a cost estimate to be able to make a fair comparison with other systems. Such a cost estimate has not been done in this study. A significant drawback of these hybrid cycles in that respect is the complex nature of the systems that will have a negative effect on the economy.

10 SPACE HEATING AND COOLING/HEAT PUMPS

10/00245 A model-based fault detection and diagnosis strategy for HVAC systems

Zhou, Q. *et al. International Journal of Energy Research*, 2009, 33, (10), 903–918.

A strategy of fault detection and diagnosis (FDD) for HVAC sub-systems at the system level is presented in this paper. In the strategy, performance indices (PIs) are proposed to indicate the health condition of different sub-systems including cooling tower system, chiller system, secondary pump systems before heat exchangers, heat exchanger system and secondary pump system after heat exchangers. The regression models are used to estimate the PIs as benchmarks for comparison with monitored PIs. The online adaptive threshold determined by training data and monitored data is used to determine whether the PI residuals between the estimation and calculation or monitoring are in the normal working range. A dynamic simulation platform is used to simulate the faults of different sub-systems and generate data for training and validation. The proposed FDD strategy is validated using the simulation data and proven to be effective in the FDD of heating, ventilating and air-conditioning (HVAC) sub-systems.

10/00246 A review on reduction method for heat and mass transfer characteristics of fin-and-tube heat exchangers under dehumidifying conditions

Pirompugd, W. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (9–10), 2370–2378.

This paper presents a review of the data reduction method for heat and mass transfer characteristics of fin-and-tube heat exchangers with dehumidification. There are many reduction methods for fin-and-tube heat exchangers under dehumidifying conditions. The data reduction methods being reviewed includes the original Threlkeld method, direct method, the equivalent dry-bulb method, tube by tube method, the fully wet and fully dry tiny circular fin method, and the finite circular fin method. Among these methods, the original Threlkeld method, direct method, the equivalent dry-bulb method are lumped method while others can divide the fin-and-tube heat exchangers into small segments for more accuracy in handling the surfaces to be fully dry, fully wet, or partially wet. In addition, the mass transfer characteristics can be obtained from the modified process line equation incorporated with the preceding methods. It should be noted that the conventional assumption of constant ratio ($h_{c,o}/h_{d,o}C_{p,a} \approx$ constant) is actually incorrect. This present paper can be used as the first guideline for the researcher for reducing the experimental data for fin-and-tube heat exchangers under dehumidifying conditions.

10/00247 CFD modelling and experimental validation of sulfur trioxide decomposition in bayonet type heat exchanger and chemical decomposer for different packed bed designs

Nagarajan, V. *et al. International Journal of Hydrogen Energy*, 2009, 34, (6), 2543–2557.

The growth of global energy demand during the 21st century, combined with the necessity to master greenhouse gas emissions has lead to the introduction of a new and universal energy carrier: hydrogen. The Department of Energy (DOE) Nuclear Hydrogen Initiative was investigating thermochemical cycles for hydrogen production using high-temperature heat exchangers. In this study a three-dimensional computational model of high-temperature heat exchanger and decomposer for decomposition of sulfur trioxide by the sulfur–iodine thermochemical water-splitting cycle with different packed bed designs has been done. The decomposer region of the bayonet heat exchanger also called as silicon carbide integrated decomposer (SID) is designed as the packed bed region. Cylindrical, spherical, cubical and hollow cylindrical pellets have been arranged inside the packed bed. The engineering design of the packed bed was very much influenced by the structure of the packing matrix, which was governed by the shape, dimension and the loading of the constituent particles. Staggered and regular packing methods are used for packing the pellets in the packed bed region. The numerical model is created using GAMBIT and fluid, thermal and chemical analyses were performed using FLUENT. The decomposition percentage of sulfur trioxide is found for the packed bed region with different pellets and the numerical results obtained is compared with the experimental results. A comparison is made for the decomposition percentage of SO_3 for the packed bed approach and the porous media approach.

10/00248 Computational study of metal hydride cooling system

Satheesh, A. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 3164–3172.

A computational study of a metal hydride cooling system working with $MmNi_{4.6}Al_{0.4}/MmNi_{4.6}Fe_{0.4}$ hydride pair is presented. The unsteady, two-dimensional mathematical model in an annular cylindrical configuration is solved numerically for predicting the time dependent conjugate heat and mass transfer characteristics between coupled reactors. The system of equations is solved by the fully implicit finite volume method (FVM). The effects of constant and variable wall temperature boundary conditions on the reaction bed temperature distribution, hydrogen concentration, and equilibrium pressures of the reactors are investigated. A dynamic correlation of the pressure–concentration–temperature plot is presented. At the given operating temperatures of 363/298/278 K ($T_H/T_M/T_C$), the cycle time for the constant and variable wall temperature boundary conditions of a single-stage and single-effect metal hydride system are found to be 1470.0 s and 1765.6 s, respectively. The computational results are compared with the experimental data reported in the literature for $LaNi_{4.61}Mn_{0.26}Al_{0.13}/La_{0.6}Y_{0.4}Ni_{4.8}Mn_{0.2}$ hydride pair and a good agreement between the two was observed.

10/00249 Conjugate natural convection with radiation in an enclosure

Kuznetsov, G.V. *et al.* Sheremet, M. A. *International Journal of Heat and Mass Transfer*, 2009, 52, (9–10), 2215–2223.

Convective-radiative heat transfer in an enclosure having finite thickness heat-conducting walls at local heating at the bottom of the cavity has been numerically studied. Heat exchange with an environment due to convection and radiation has been considered on one of external sides of the decision region. The effect of parameters such as the Grashof number, the transient factor, the optical thickness and the solid wall thermal conductivity both on the local thermo-hydrodynamic characteristics such as streamlines and temperature fields and on the integral parameter like the average Nusselt number on the heat source surface has been analysed.

10/00250 Effective pipe-to-borehole thermal resistance for vertical ground heat exchangers

Sharqawy, M. H. *et al. Geothermics*, 2009, 38, (2), 271–277.

The effective pipe-to-borehole thermal resistance of a vertical ground heat exchanger is investigated numerically. An analysis is carried out to determine the dimensionless geometrical parameters affecting such resistance. The heat transfer rates between the U-shaped pipes and the borehole are determined numerically and compared with some well-known limiting analytical solutions. A best-fit correlation for the effective pipe-to-borehole thermal resistance is presented in dimensionless form. The results are compared against approximate analytical solutions that represent the U-shaped pipes as a single pipe of equivalent diameter and against experimental data available in the literature. It is found that the available models do not accurately represent the effective pipe-to-borehole thermal resistance.

10/00251 Energy and exergy analyses of space heating in buildings

Yildiz, A. and Güngör, A. *Applied Energy*, 2009, 86, (10), 1939–1948.

In the present study, energy and exergy analyses are presented for the whole process of space heating in buildings. This study is based on a pre-design analysis tool, which has been produced during ongoing work for the International Energy Agency (IEA) formed within the Energy Conservation in Buildings and Community Systems Programme (ECBCSP) Annex 37. Throughout this paper, in all of the calculations such as heat losses and gains were taken according to Turkish Standards Institution TSE, which is in accordance with the European Standard TS EN ISO 13789. In the analysis, heating load is taken account but cooling load is neglected and the calculations presented here are done using steady state conditions. The analysis is applied to an office in Izmir with a volume of $720\,m^3$ and a net floor area of $240\,m^2$ as an example of application. Indoor and exterior air temperatures are 20 °C and 0 °C, respectively. It is assumed that the office is heated by a liquid natural gas (LNG) fired conventional boiler, an LNG condensing boiler and an external air–air heat pump. With this study, energy and exergy flows are investigated. Energy and exergy losses in the whole system are quantified and illustrated. The highest efficiency values in terms of energy and exergy were found to be 80.9% for external air–air heat pump and 8.69% for LNG condensing boiler, respectively.

10/00252 Enhancement of convective cooling using oscillating fins

Dey, S. and Chakrborty, D. *International Communications in Heat and Mass Transfer*, 2009, 36, (5), 508–512.

Tailoring the local flow field around a fin can substantially enhance the forced convection heat transfer from a conventional heat sink. A fin is set into oscillation leading to rupture of the thermal boundary layer developed on either side of the fin. This enhancement in heat transfer is demonstrated through an increase in the time-averaged Nusselt Number (Nu) on the fin surfaces. Nu has been found to be strongly dependent on the flow Reynolds Number (Re), the frequency and amplitude of the fin oscillations. A threshold amplitude and frequency is identified beyond which Nu improvements are observed for fixed Re.

10/00253 Environmental performance and economic analysis of all-variable speed chiller systems with load-based speed control

Yu, F. W. and Chan, K. T. *Applied Thermal Engineering*, 2009, 29, (8–9), 1721–1729.

There are increasing views on implementing all-variable speed chiller plants in place of conventional constant speed plants. Supporters of these views claim that all-variable speed chiller systems can operate much more efficiently at part load in response to changes in building cooling load. This paper introduces load-based speed control for all-variable speed plants to optimize their environmental performance. Thermodynamic-behaviour chiller system models were developed to perform environmental assessment (in terms of annual electricity and water consumption) for typical constant speed and all-variable speed chiller systems operating for the cooling load profile of a local office building. Operating cost differences between the two systems were calculated and compared in an economic analysis. Applying load-based speed control to the variable speed chiller plant can decrease the annual total electricity use by 19.7% and annual water use by 15.9% relative to the corresponding constant speed plant. The significance of this study is to provide more insights into how to make chiller systems more sustainable.

10/00254 Evaluation of environmental and physiological factors of a whole ceiling-type air conditioner using a salivary biomarker

Tahara, Y. *et al. Building and Environment*, 2009, 44, (6), 1156–1161.

In order to improve environmental condition such as humidity and airflow in living spaces, a whole ceiling-type air conditioner is proposed. This novel air conditioner exhaust dispersed airflow from the whole ceiling by using a three-dimensional knit fabric. The purpose of this paper is to reveal the effects when controlling humidity and airflow using the whole ceiling-type air conditioner compared to a commercialized concentrated exhaust air conditioner (normal-type air conditioner) under the same temperature. Salivary α-amylase activity (SAA) was used as an index of sympathetic nervous activity. An acute experiment for a 15 min period was conducted using 12 healthy young female adults. No significant differences in room and skin temperatures were observed between the whole ceiling-type air conditioner and the normal-type air conditioner. The whole ceiling-type air conditioner showed 11.1% lower humidity than the normal-type air conditioner. The whole ceiling-type air conditioner showed one-thirteenth the airflow of the normal-type air conditioner. As a result, the PMV of the whole ceiling-type air conditioner was more comfortable level than the normal one. Moreover, subjective evaluation questionnaire revealed a significant difference was observed in wind perception (windy). The

SAA of subjects under the whole ceiling-type air conditioner showed significantly low values compared with the normal-type air conditioner. It was found that the subject's sympathetic nervous activity has been inactivated under the conditions of the whole ceiling-type air conditioner. Thus, it was revealed that the whole ceiling-type air conditioner provides a more comfortable air environment by reducing physical stimulations to humans.

10/00255 Experimental approach to the contribution of plant-covered walls to the thermal behaviour of building envelopes

Eumorfopoulou, E. A. and Kontoleon, K. J. *Building and Environment*, 2009, 44, (5), 1024–1038.

The use of vegetation has an important impact on the thermal performance of buildings and on the modification of the urban climate as well, both in winter and summer. Plants absorb a significant amount of solar radiation for their growth and biological functions, functioning as a solar barrier that prevents solar radiation absorption extensively. Their utilization is essential and can considerably improve the microclimate of the built environment. Vegetation planted to cover the external surface of a building is common practice in urban areas. However, up to now, it has not been fully approved as an energy-saving method. Climbers can provide a cooling potential on the building surface, which is very important during the hot periods of the year, especially in warm climates. Hence, the peak temperatures that appear are essentially lower, in addition to the decrease of heat flow losses. In this study the thermal analysis concerns two equivalent building floors that incorporate non-covered and covered with plants wall sections (insulated wall surfaces), respectively. The investigation is carried out during the cooling period in the Greek region. A comparison between the bare and plant-covered surface sections of the walls is conducted via an experimental setup (stationary method). Results are focused on the developed temperature variations and dynamic thermal characteristics of wall surfaces for both cases under investigation. As it is shown, the contribution of plant-covered wall sections is important so that the thermal behaviour of the building envelope can be improved.

10/00256 Experimental assessment of a phase change material for wall building use

Kuznik, F. and Virgone, J. *Applied Energy*, 2009, 86, (10), 2038–2046.

The thermal performances of a phase change material (PCM) copolymer composite wallboard has been experimentally investigated in a full scale test room. The test cell is totally controlled so that a typical day can be repeated (temperature and solar radiative flux). Effects of the PCM are investigated comparing the results obtained with and without composite wallboards for three cases: a summer day, a winter day and a mid-season day. The results show that: (1) for all the cases tested, the decrement factor varies between 0.73 and 0.78 which is quite interesting for use in buildings and particularly for renovation; (2) the air temperature in the room with PCM lowers up to 4.2°, the comfort enhancement is more important if the surface temperatures are also considered; (3) the PCM wallboards enhance the natural convection in the room and then there is no thermal stratification contrary to the room without composite; (4) the numerical experiments are fully described and can then be used to evaluate PCM numerical modelling.

10/00257 Frost behavior on a fin considering the heat conduction of heat exchanger fins

Kim, J.-S. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2581–2588.

A mathematical model is proposed for predicting frost behaviour on a heat exchanger fin under frosting conditions, taking into account fin heat conduction. The change in the three-dimensional airside airflow caused by frost growth is reflected in this model. The numerical estimates of frost thickness are consistent with experimental data, with an error of less than 10%. Due to fin heat conduction, frost thickness decreases exponentially toward the fin tip, while considerable frost growth occurs near the fin base. When a constant fin surface temperature is assumed, the predicted frost thickness was larger by more than 200% at maximum, and the heat flux by more than 10% on average, compared to results obtained with fin heat conduction taken into account. Therefore, fin heat conduction could be an essential factor in accurately predicting frost behaviour. To improve prediction accuracy under the assumption of constant fin surface temperature, the equivalent temperature (for predicting frost behaviour) is defined to be the temperature at which the heat transfer rate neglecting fin heat conduction is the same as the heat transfer rate with fin heat conduction taken into consideration. Finally, a correlation for predicting the equivalent temperature is suggested.

10/00258 Fuel cells for micro-combined heat and power generation

Hawkes, A. *et al. Energy Environmental Science*, 2009, 2, (7), 729–744.

Micro-combined heat and power (CHP) holds great potential for lowering energy cost and CO_2 emissions in the residential housing sector. Of the various micro-CHP technologies, fuel cells, and in particular solid oxide fuel cells, show great promise due to their high electrical efficiency and resulting low heat-to-power ratio that is better suited to residential applications. However, fuel cells are still under development and the capital cost of units available today remains high. This paper looks at the technological aspects and operating modes of fuel cells relevant to micro-CHP as well as examining the state of commercial development, life cycle issues and the techno-economics of fuel cells for micro-CHP at the residential scale.

10/00259 Heat conduction with seasonal freezing and thawing in an active layer near a tower foundation

Duan, X. and Naterer, G. F. *International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 2068–2078.

In this paper, seasonal freezing and thawing of an active layer near a power transmission tower foundation are investigated experimentally with a metal rod buried in an enclosure filled with soil. The measured soil temperatures are used to examine thermal effects of the tower footing and snow cover on seasonal freezing and thawing cycles. It was found that the metal tower has significant thermal effects on the local region around the tower footing. This increases the thaw depth of the active layer and lengthens the freezing/thawing cycle, which adversely affects the foundation stability and safety. These results provide useful new insight of practical utility in the design and maintenance of power transmission line foundations and other infrastructure in northern regions.

10/00260 Heat flux estimation of a plasma rocket helicon source by solution of the inverse heat conduction problem

Mulcahy, J. M. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (9–10), 2343–2357.

A solution of the inverse heat conduction problem (IHCP) by the steepest descent method is carried out in order to determine the waste heat flux from a helicon plasma discharge using transient surface temperature measurements obtained from infrared thermography. The infrared camera data is calibrated against thermocouple data and mapped to real locations on the observed surface. The magnitude and distribution of the heat flux to the gas containment tube in the helicon is investigated as the applied power, gas flow rate, magnetic field distribution and neutral gas are varied.

10/00261 Heat transfer by natural convection, conduction and radiation in an inclined square enclosure bounded with a solid wall

Nouanegue, H. F. *et al. International Journal of Thermal Sciences*, 2009, 48, (5), 871–880.

In this paper, conjugate heat transfer by natural convection, conduction and radiation is studied in an inclined square enclosure bounded by a solid wall with its outer boundary at constant temperature while the opposing active wall is with a constant heat flux. The authors solved two-dimensional coupled equations of conservation of mass, momentum and energy, with the Boussinesq approximation using finite difference method and the SIMPLER algorithm. Various parameters were: Rayleigh number from 10^8 to 3×10^{10}, dimensionless conductivity of bounding wall from 10 to 40 and dimensionless wall width from 0 to 0.15, aspect ratio equal to 1, the inclination angle 60 to 150° and the surface emissivity from 0 to 1. The results were presented in terms of heat flux and Nusselt number as a function of the Rayleigh number and other dimensionless parameters, as well as in terms of flow and temperature fields. It was found that the interaction among the three modes of heat transfer was significant, the influence of the surface radiation on the natural convection was non-negligible and the flow and temperature fields as well as the heat transfer across the enclosure were modified.

10/00262 Heat transfer studies on a generator-absorber-exchange absorption compression (GAXAC) cooler

Rameshkumar, A. *et al. Applied Energy*, 2009, 86, (10), 2056–2064.

A detailed heat transfer model of generator-absorber-exchange absorption compression cycle using ammonia–water as working fluid is reported. The effect of UA (heat transfer conductance, kW/K) of each component on COP and cycle capacity is investigated. The results show that UA of the absorber and high temperature generator have significant impact on COP and cycle capacity. For a capacity of 11.56 kW, the maximized COP with minimum UA value for all heat exchanging components is found to be 1.185. Further the effect of mass flow rate and inlet temperatures of hot fluid, chilled water and cooling water are also investigated.

10/00263 High pressure cryo-storage of hydrogen by adsorption at 77 K and up to 50 MPa

Weinberger, B. and Lamari, F. D. *International Journal of Hydrogen Energy*, 2009, 34, (7), 3058–3064.

This paper focuses on hydrogen adsorption on large surface area solids, combining optimal extreme conditions, i.e. very high pressure and low temperature for gas storage process purpose. Therefore, a new volumetric device is elaborated to obtain excess adsorption isotherms at 77 K up to 500 bar. Two activated carbons with different microporosities are analysed in the view of hydrogen storage investigation. Also, the results are compared to zeolite adsorption properties. Based on these results, the total mass and volumetric storage capacity are calculated using the bulk density relationship. Thereby, high storage *in situ* capacities were obtained equal to 5.2 wt% and 54.5 kgH_2/m^3. Further, the authors also considered practical application aspects related to hydrogen storage process in highly porous packed materials.

10/00264 Instability phenomena in a two-phase microchannel thermosyphon

Garrity, P. T. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1701–1708.

The behaviour of a two-phase thermosyphon, consisting of a microchannel evaporator plate and a condenser, is investigated to gain insight into the system limiting instability. A microchannel plate has been fabricated with 56 square channels that have a 1 × 1 mm cross section and a length of 115 mm. Experiments have been conducted for various condenser heights with the heat flux as the control variable. A step increase in heat flux is used to quantify the response of the system, including variations in mass flow rate, temperature, and pressure drop. Results show that small fluctuations about the steady state give rise to the instability for situations with a uniform heat load. A predictive model based on the momentum equation is introduced to estimate the onset of instability, and the threshold heat flux is predicted to within ±10% uncertainty.

10/00265 Integration of the solar thermal energy in the construction: analysis of the solar-assisted air-conditioning system installed in CIESOL building

Rosiek, S. and Batlles, F. J. *Renewable Energy*, 2009, 34, (6), 1423–1431.

In the last few years the solar-powered air-conditioning systems have been in intensive development and more often are considered as the viable application for the thermal solar systems in the regions of southern Europe. This is mainly due to the increasing higher electrical consumption in many countries (especially in Spain), which is moving from the winter to summer months due to expanding usage of cooling systems in this period of the year. In this paper, the behaviour of the solar-assisted air-conditioning system installed in the CIESOL building will be analysed. This system consists mainly of flat-plate solar collectors and the simple effect LiBr–H_2O absorption chiller. Different operation modes were analysed. Coefficient of performance (COP) at various generator, absorber, condenser and evaporator temperatures is investigated and experimental results show that in practice it is easy to obtain values of about 0.6. The main goal of this paper is to describe the characteristics of the developing building and the solar-assisted air-conditioning system. Another useful purpose is to find the optimum conditions and operation parameters for the solar system through analysing various systems' operation strategies.

10/00266 Inverse estimation for the unknown frost geometry on the external wall of a forced-convection pipe

Chen, W.-L. and Yang, Y.-C. *Energy Conversion and Management*, 2009, 50, (6), 1457–1464.

In this study, a conjugate gradient method based inverse algorithm is applied to estimate the unknown frost-layer boundary profile on the external wall of a pipe system using temperature measurements. It is assumed that no prior information is available on the functional form of the unknown profile; hence the procedure is classified as the function estimation in inverse calculation. The temperature data obtained from the direct problem are used to simulate the temperature measurements. The accuracy of the inverse analysis is examined by using simulated exact and inexact temperature measurements. Results show that an excellent estimation on boundary profile can be obtained for the test case considered in this study.

10/00267 Inverse problem of transpiration cooling for estimating wall heat flux by LTNE model and CGM method

Shi, J. and Wang, J. *International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2714–2720.

In this work, a transient inverse problem of transpiration cooling is investigated in detail. The heat flux on the wall to be cooled is estimated by single point temperature measurement. The local thermal non-equilibrium (LTNE) model is utilized to describe the energy conservation of transpiration cooling process, and the conjugate gradient method (CGM) is extended to solve the inverse problem. The accuracy of the solutions of the inverse problem is examined through three given heat fluxes with given measurement errors. The examination shows that with the LTNE model and CGM, satisfactory solutions can be obtained. The influences of the variation in thermal properties, compressibility and the location of sensor on the accuracy of the solutions are analysed. The analysis indicates that the variation in thermal properties and compressibility should be considered when a large temperature gradient exists, and the sensor location should be as close as possible to the hot wall. The inverse solutions obtained by the measurements of solid and fluid temperatures are compared. Through the comparison, it is found that using the solid temperature measurement as the input of the inverse problem is better than using the fluid temperature measurement.

10/00268 Investigation of energy transportation capability of a phase change slurry through a cold storage-cooling coil system

Ma, X. *et al. International Journal of Energy Research*, 2009, 33, (11), 999–1004.

Microencapsulated phase change materials slurries (MEPCM slurries) have the advantage that they can be used as heat transport and storage medium, and therefore provide improved continuity of energy transport. Energy transportation capability of a MEPCM slurry based on Rubitherm RT6 through a cold storage-air handling system was investigated for various concentrations and pump powers. The transport properties of the MEPCM have been identified. The optimum concentration for maximum energy transportation capability and energy transportation effectiveness of the system has been found. This investigation is intended for determination of the optimum concentration of MEPCM slurry for an air conditioning system that uses MEPCM slurry as a secondary cooling medium directly into air handling units and stored for load shifting.

10/00269 Investigation on heat transfer and pressure drop during swirl flow boiling of R-134a in a horizontal tube

Akhavan-Behabadi, M. A. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1918–1927.

An experimental investigation has been carried out to study the effect of twisted tape inserts on heat transfer enhancement and pressure drop in a horizontal tube during swirl flow boiling of R-134a. The test-evaporator was an electrically heated horizontal copper tube and twisted tapes with different twist ratios of 6, 9, 12 and 15 were inserted one by one. The data were acquired at the refrigerant mass velocities of 54, 86, 114 and 136 $kg/s\,m^2$. The twisted tape inserts increases the boiling heat transfer coefficients and the pressure drop across the test-evaporator. An empirical correlation has also been developed to predict the swirl flow pressure drop in the test-evaporator.

10/00270 Kinetics of water adsorption/desorption under isobaric stages of adsorption heat transformers: The effect of isobar shape

Glaznev, I. S. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1774–1777.

Effect of the shape of equilibrium adsorption isobar on dynamics of water adsorption/desorption under isobaric stages of a basic cycle of an adsorption heat transformer has been studied. Selective water sorbent SWS-1L ($CaCl_2$ confined to mesoporous silica gel) was used for these tests as its water adsorption isobars have segments with both convex and concave shapes. From these experiments the conclusion has been drawn that the dynamics of adsorption on a single adsorbent grain is closely linked with the shape (convex or concave) of the segment of water adsorption isobar between initial and final temperatures of the isobaric process. In particular, under the same boundary conditions desorption is faster than adsorption for a concave isobar segment and vice versa for a convex one.

10/00271 Local asymptotic stability of an irreversible heat pump subject to total thermal conductance constraint

Huang, Y. *Energy Conversion and Management*, 2009, 50, (6), 1444–1449.

The local asymptotic stability of an irreversible heat pump subject to the total thermal conductance constraint is investigated based on the stability criteria for almost linear systems. An irreversible heat pump system that is modelled by the differential equation expresses the rate of change of the temperatures of the working fluid in the heat addition and heat rejection processes. From the local stability analysis, it is found that a critical point of an almost linear system is asymptotically stable. After an arbitrarily small perturbation, the system state exponentially decays to an asymptotically stable critical point with either of two characteristic relaxation times that are a function of the total thermal conductance UA, thermal conductance allocation ratio ϕ, heat capacity C, internal irreversible factor I, temperature of the heat reservoir T_H and heating load Q. The behaviour of solutions of the system is presented qualitatively by sketching its phase portrait. One eigendirection in a phase portrait is the non-zero constant vector, and the other is a function of UA, ϕ, I, Q_H, T_H and T_L. Finally, the local asymptotic stability and steady state energetic properties of the irreversible heat pump are discussed.

10/00272 Low-temperature lattice thermal conductivity in free-standing GaN thin films

Kamatagi, M. D. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, 2885–2892.

Low-temperature ($2 < T < 100\,\mathrm{K}$) lattice thermal conductivity, κ_p in a semiconducting free-standing thin film (FSTF) is studied using a modified Callaway model. The quantization of acoustic phonons in FSTFs is taken into account and explicit contributions to κ_p from the shear, dilatational and flexural modes of the confined acoustic phonons are considered. The scattering of phonons is assumed to be by sample boundaries, impurities, dislocations and other phonons via both normal and umklapp processes. Numerical results are presented for the GaN system. The phonon confinement effect, the sample finite size effect and the relative importance of confined phonon modes are investigated. The role of dislocations in limiting κ_p is also discussed. Results are compared with those based on bulk description of acoustic phonons; bulk phonons are found to underestimate (overestimate) κ_p in the boundary scattering regime (at higher temperatures). The calculations demonstrate that low-temperature thermal conductivity studies can lead to a better understanding of phonon scattering in FSTFs.

10/00273 Magnetoconvection in an enclosure of water near its density maximum with Soret and Dufour effects

Nithyadevi, N. and Yang, R.-J. *International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1667–1676.

In this paper, unsteady double-diffusive magnetoconvection of water in an enclosure with Soret and Dufour effects around the density maximum has been numerically investigated. The right vertical wall has constant temperature, θ_c, while the left vertical wall is θ_h, with $\theta_h > \theta_c$. The concentration in right wall is maintained lower than left wall ($c_h > c_c$). The remaining horizontal walls are adiabatic. The governing equations are solved by control volume method using the SIMPLE algorithm with QUICK scheme. Representative results illustrating the effects of the thermal Rayleigh number, Hartmann number, the direction of magnetic field, density inversion parameter, buoyancy ratio, Schmidt number, and Soret and Dufour parameters on the contour maps of the fluid flow, temperature and concentration as well as the profile of velocity at mid-section of the enclosure are reported. In addition, numerical results for the average Nusselt and Sherwood numbers are presented for various parametric conditions and discussed.

10/00274 Micro thermoelectric cooler: planar multistage

Hwang, G. S. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1843–1852.

A suspended, planar multistage micro thermoelectric (TE) cooler is designed using thermal network model to cool microelectromechanical systems (MEMS) devices. Though the planar (two-dimensional) design is compatible with MEMS fabrication, its cooling performance is reduced compared to that of a pyramid (three-dimensional) design, due to a mechanically indispensable thin dielectric substrate (SiO_2) and technical limit on TE film thickness. The authors optimized the planar, six-stage TE cooler for maximum cooling, and predicted $\Delta T_{\max} = 51\,\mathrm{K}$ with power consumption of 68 mW using undoped, patterned 4–10 μm thick co-evaporated Bi_2Te_3 and Sb_2Te_3 films. Improvement steps of the planar design for achieving cooling performance of the ideal pyramid design are discussed in this paper. The predicted performance of a fabricated prototype is compared with experimental results with good agreements.

10/00275 Model of a solar driven steam jet ejector chiller and investigation of its dynamic operational behaviour

Pollerberg, C. *et al. Solar Energy*, 2009, 83, (5), 732–742.

The solar driven steam jet ejector chiller (SJEC) is a new device for solar air-conditioning. Previously, solar SJEC has been only investigated theoretically by static models and practically by small test rigs. A demonstration plant does not exist so far, so that the operational behaviour of a solar SJEC has not been investigated in detail yet. But due to the fact that solar irradiation and cold demand are not constant, the operational behaviour is very important for the plant design and the controlling concept. This publication presents a model for a SJEC and the results of dynamic simulations. The proposed model allows creating and investigating different plant concepts by its structure in model components. After the validation of the model, simulations of a fictive solar SJEC with parabolic trough collectors are accomplished to analyse the dynamic operational behaviour of a future plant.

10/00276 Modelling and performance study of a continuous adsorption refrigeration system driven by parabolic trough solar collector

El Fadar, A. *et al. Solar Energy*, 2009, 83, (6), 850–861.

This article suggests a numerical study of a continuous adsorption refrigeration system consisting of two adsorbent beds and powered by parabolic trough solar collector (PTC). Activated carbon as adsorbent and ammonia as refrigerant are selected. A predictive model accounting for heat balance in the solar collector components and instantaneous heat and mass transfer in adsorbent bed is presented. The validity of the theoretical model has been tested by comparison with experimental data of the temperature evolution within the adsorber during isosteric heating phase. A good agreement is obtained. The system performance is assessed in terms of specific cooling power (SCP), refrigeration cycle COP (COP_{cycle}) and solar coefficient of performance (COP_s), which were evaluated by a cycle simulation computer program. The temperature, pressure and adsorbed mass profiles in the two adsorbers have been shown. The influences of some important operating and design parameters on the system performance have been analysed. The study has put in evidence the ability of such a system to achieve a promising performance and to overcome the intermittence of the adsorption refrigeration systems driven by solar energy. Under the climatic conditions of daily solar radiation being about 14 MJ per $0.8\,\mathrm{m}^2$ ($17.5\,\mathrm{MJ/m}^2$) and operating conditions of evaporating temperature, $T_{ev} = 0\,^\circ\mathrm{C}$, condensing temperature, $T_{con} = 30\,^\circ\mathrm{C}$ and heat source temperature of 100 °C, the results indicate that the system could achieve a SCP of the order of 104 W/kg, a refrigeration cycle COP of 0.43, and it could produce a daily useful cooling of 2515 kJ per $0.8\,\mathrm{m}^2$ of collector area, while its gross solar COP could reach 0.18.

10/00277 Molecular dynamics simulation of thermal conductivity of nanocrystalline composite films

Roberts, N. A. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 2002–2008.

The efficiency of a thermoelectric material is measured by the figure of merit ZT, which is inversely proportional to the thermal conductivity. Superlattice structures often have a reduced thermal conductivity because of the introduction of interface scattering and, therefore, improved performance. The present work is focused on the effective thermal conductivity of nanocomposite films. This configuration could also improve ZT because of phonon-interface scattering introduced by the nanocrystals. The effects of crystal size and mass fraction are studied numerically using a molecular dynamics simulation. Results indicate that a reduction of 25% in the effective thermal conductivity can be achieved with the addition of nanocrystals which is comparable to that found in experimental measurement. However, the effective thermal conductivity was never reduced below the alloy limit.

10/00278 Natural convection heat transfer from a horizontal isothermal elliptical cylinder with internal heat generation

Cheng, C.-Y. *International Communications in Heat and Mass Transfer*, 2009, 36, (4), 346–350.

This work examines the natural convection heat transfer from a horizontal isothermal cylinder of elliptic cross-section in a Newtonian fluid with temperature-dependent internal heat generation. The governing boundary layer equations are transformed into a non-dimensional form and the resulting nonlinear systems of partial differential equations are solved numerically applying cubic spline collocation method. Results for the local Nusselt number and the local skin-friction coefficient are presented as functions of eccentric angle for various values of heat generation parameters, Prandtl numbers and aspect ratios. Results show that both the heat transfer rate and skin friction of the elliptical cylinder with slender orientation are higher than the elliptical cylinder with blunt orientation. Moreover, an increase in the heat generation parameter for natural convection flow over an isothermal horizontal elliptic cylinder leads to a decrease in the heat transfer rate from the elliptical cylinder and an increase in the skin friction of the elliptical cylinder.

10/00279 Numerical investigation of heat transfer and pressure drop characteristics of tube–fin heat exchangers in ice slurry HVAC system

Kalaiselvam, S. *et al. Applied Thermal Engineering*, 2009, 29, (8–9), 1831–1839.

This paper analyses the heat transfer and pressure drop characteristics of a tube–fin heat exchanger in ice slurry HVAC system. Ice slurry is a suspension of crystallized water-based ice solution with a freezing point depressant like ethylene glycol. The ice-slurry is pumpable, hence it is also called pumpable ice. The composition of ice slurry considered for analysis is 14% ice fraction, 16% ethylene glycol, and 70% water by volume. It is deduced that the ice slurry HVAC system results in 7.4% increase in temperature drop over the conventional chilled water system The latent heat absorbed by ice slurry on melting makes it an attractive choice for achieving high degree of cooling. The numerical analysis was conducted by simulating the ice slurry tube flow region and air flow region of tube–fin heat exchanger in the air-handling unit of HVAC system. For the simulation six different louver patterns with 10 to 55 louver angle were considered. The design of the tube–fin heat exchanger for optimal heat transfer and pressure drop characteristics was also determined with the optimization parameter like louver angle, fin pitch, and ice slurry flow velocity.

10/00280 Numerical modelling of heat and mass transfer in finned dehumidifier

Croce, G. *et al. Applied Thermal Engineering*, 2009, 29, (7), 1366–1374.

In several heat exchange devices, phase transition occurs in a small region adjacent to the wall, and the secondary phase is present only in a thin layer running along the wall, allowing for decoupling between the fluid dynamic computation of the core flow and the numerical analysis of the secondary phase. This happens in finned dehumidifier, but also in spray cooling or defogging problems. In a finned dehumidifier, or in air conditioning evaporators, the secondary phase is provided by moist air condensation, and may consist of discrete droplets, continuous film or a collection of rivulets. Several levels of approximation may be adopted, depending on the specific problem: perfect drain assumption requires only the addition of a heat source in the energy equation, otherwise the water layer behaviour has to be taken into account. Furthermore, a heat and mass transfer analogy may or may not be appropriate; in the latter case, the solution of the diffusion equation of humidity is required. Here, different levels of approximation are compared with literature experimental data for condensation over a vertical fin. Results show that thermal resistance and gravity effects, in the considered geometry, are negligible, and the condensate takes the form of a collection of still droplets, rather than a flowing film. This has an effect on the actual heat transfer and water layer build-up, and the variation of temperature along the fin induces some discrepancy with respect to the straightforward application of the heat and mass transfer analogy.

10/00281 Optimal design of a forced circulation solar water heating system for a residential unit in cold climate using TRNSYS

Hobbi, A. and Siddiqui, K. *Solar Energy*, 2009, 83, (5), 700–714.

An indirect forced circulation solar water heating systems using a flat-plate collector is modelled for domestic hot water requirements of a single-family residential unit in Montreal, Canada. All necessary design parameters are studied and the optimum values are determined using TRNSYS simulation program. The solar fraction of the entire system is used as the optimization parameter. Design parameters of both the system and the collector were optimized that include collector area, fluid type, collector mass flow rate, storage tank volume and height, heat exchanger effectiveness, size and length of connecting pipes, absorber plate material and thickness, number and size of the riser tubes, tube spacing, and the collector's aspect ratio. The results show that by utilizing solar energy, the designed system could provide 83–97% and 30–62% of the hot water demands in summer and winter, respectively. It is also determined that even a locally made non-selective-coated collector can supply about 54% of the annual water heating energy requirement by solar energy.

10/00282 Performance characteristics of pulsating heat pipes as integral thermal spreaders

Yang, H. *et al. International Journal of Thermal Sciences*, 2009, 48, (4), 815–824.

In the recent past, pulsating heat pipes have attracted the attention of many researchers as viable candidates for enhanced heat transfer through passive two-phase heat transfer mechanism. Although a complete theoretical understanding of operational characteristics of this device is not yet achieved, there are many emerging niche applications, ranging from electronics thermal management to compact heat exchangers. For a better theoretical understanding, it is vital to generate experimental data under various operating boundary conditions. In this background, this paper presents an experimental study on two flat plate closed loop pulsating heat pipes in a thermal spreader configuration. Both are made of aluminium with overall size $180\times120\times3\,\text{mm}^3$; one structure having 40 parallel square channels with cross-section $2\times2\,\text{mm}^2$, while the second with 66 parallel square channels with cross-section $1\times1\,\text{mm}^2$. The working fluid employed was Ethanol. Some peculiar performance trends, in comparison with circular channel devices, have been observed which are attributed to the sharp angled corners of the channels. The influence of various operating parameters, including volumetric filling ratio of the working fluid, input heat flux and operating orientation, on the thermo-hydrodynamic performance, was investigated. Successful operation at all orientations with respect to gravity was also achieved. In terms of applications, this paper explores the possibility of embedded pulsating heat pipe as an integrated structure or heat spreader, so as to render higher overall thermal conductance to the host substrate.

10/00283 Performance evaluation of mixed convection in an inclined square channel with uniform temperature walls

Ichimiya, K. and Matsushima, Y. *International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1802–1810.

Numerical analyses were performed for the effect of inclined angle on the mixing flow in a square channel with uniform temperature walls ($T_w = 30\,^\circ\text{C}$) and inlet temperature ($T_0 = 10\,^\circ\text{C}$). Three-dimensional governing equations were solved numerically for $Re = 100$, $Pr = 0.72$ and various inclined angles (from -90° to 90°). Three-dimensional behaviour of fluid in a channel was examined for each angle. Thermal performance was evaluated using the relationship between Nusselt number ratio and pressure loss ratio with and without buoyancy induced flow as a parameter of inclined angles. High heat transfer and low pressure loss region was from -15° to -60° in thermal performance using mean Nusselt number ratio.

10/00284 Preparation and thermophysical properties of nanoparticle-in-paraffin emulsion as phase change material

Ho, C. J. and Gao, J. Y. *International Communications in Heat and Mass Transfer*, 2009, 36, (5), 467–470.

In this study, phase change material (PCM) embedded by nanoparticles was prepared by emulsifying alumina (Al_2O_3) nanoparticles in paraffin (n-octadecane) by means of a non-ionic surfactant. The formulated nanoparticle-in-paraffin emulsions contain the nanoparticles of 5 wt% and 10 wt%, respectively; their effective thermophysical properties, such as latent heat of fusion, density, dynamic viscosity, and thermal conductivity, were investigated experimentally. The experimentally measured density of the emulsions agrees excellently with that predicted based on the mixture theory. The measured thermal conductivity and dynamic viscosity for the nanoparticle-in-paraffin emulsions formulated show a nonlinear increase with the mass fraction of the nanoparticles compared with that for the pure paraffin, depending on the temperature.

10/00285 Preparation, thermal properties and thermal reliability of palmitic acid/expanded graphite composite as form-stable PCM for thermal energy storage

Sari, A. and Karaipekli, A. *Solar Energy Materials and Solar Cells*, 2009, 93, (5), 571–576.

This study is focused on the preparation and characterization of thermal properties and thermal reliability of palmitic acid (PA)/expanded graphite (EG) composite as form-stable phase change material (PCM). The maximum mass fraction of PA retained in EG was found as 80 wt% without the leakage of PA in melted state even when it is heated over the melting point of PA. Therefore, the PA/EG (80/20 w/w%) composite was characterized as form-stable PCM. From differential scanning calorimetry (DSC) analysis, the melting and freezing temperatures and latent heats of the form-stable PCM were measured as 60.88 and 60.81 °C and 148.36 and 149.66 J/g, respectively. Thermal cycling test showed that the composite PCM has good thermal reliability although it was subjected to 3000 melting/freezing cycles. Fourier transformation infrared (FT-IR) spectroscopic investigation indicated that it has good chemical stability after thermal cycling. Thermal conductivities of PA/EG composites including different mass fractions of EG (5%, 10%, 15% and 20%) were also measured. Thermal conductivity of form-stable PA/EG (80/20 w/w%) composite (0.60 W/mK) was found to be 2.5 times higher than that of pure PA (0.17 W/mK). Moreover, the increase in thermal conductivity of PA was confirmed by comparison of the melting and freezing times of pure PA with that of form-stable composite. Based on all results, it was concluded that the form-stable PA/EG (80/20 w/w%) has considerable latent heat energy storage potential because of its good thermal properties, thermal and chemical reliability and thermal conductivity.

10/00286 Roughness and surface material effects on nucleate boiling heat transfer from cylindrical surfaces to refrigerants R-134a and R-123

Jabardo, J. M. S. *et al. Experimental Thermal and Fluid Science*, 2009, 33, (4), 579–590.

This paper presents the results of an experimental investigation carried out into the effects of the surface roughness of different materials on nucleate boiling heat transfer of refrigerants R-134a and R-123. Experiments have been performed over cylindrical surfaces of copper, brass and stainless steel. Surfaces have been treated by different methods in order to obtain an average roughness, Ra, varying from 0.03 µm to 10.5 µm. Boiling curves at different reduced pressures have been raised as part of the investigation. The obtained results have shown significant effects of the surface material, with brass being the best performing and stainless steel the worst. Polished surfaces seem to present slightly better performance than the sand paper roughened. Boiling on very rough surfaces presents a peculiar behaviour characterized by good thermal performance at low heat fluxes, the performance deteriorating at high heat fluxes with respect to smoother surfaces.

10/00287 Sorption heat pumping technologies: comparisons and challenges

Ziegler, F. *International Journal of Refrigeration*, 2009, 32, (4), 566–576.

Heat pumping devices which are operating on sorption effects comprise at least two times two categories, namely liquid or solid sorption cycles on the one hand, and open or closed cycles on the other hand. For the benefit of energy saving and the environment as well as for the further development of the technology it is important to be able to compare and evaluate these options in the context of the respective application. Some ideas to this end are shown in this paper. First the meaning of temperatures and humidity for the difference between open and closed systems is discussed, and there are a lot of similarities. Then some differences between solid and liquid sorption which are especially important for the question of minimum operating temperature and part load behaviour are being reviewed, and it is found that there is something to learn, mutually. Finally the consequences of solar fraction, auxiliary power consumption, and cogeneration efficiency are being highlighted, in order to check the perception of sorption systems to be environmentally benign. These consequences are important for all kinds of sorption cooling systems. It can be expected that there are significant improvements in the efficiency of power plants and compression cooling systems; consequently it is found that sorption technology must improve its performance considerably also in order to stay competitive.

10/00288 Study on medium-temperature chemical heat storage using mixed hydroxides

Kato, Y. *et al. International Journal of Refrigeration*, 2009, 32, (4), 661–666.

It was demonstrated that chemical heat storage materials mixed with metal hydroxides were capable of storing heat at medium temperatures of approximately 200–300 °C. The performances of the developed materials were demonstrated in a thermo-balance and packed bed reactor. The mixed hydroxides can increase the operation heat storage temperature by changing the composition of mixed metal oxides in the material. $\mathrm{Mg}_{\alpha}\mathrm{Ni}_{1-}\alpha(\mathrm{OH})_2$, which is a mixed hydroxide of magnesium hydroxide, $Mg(OH)_2$, and nickel hydroxide, $Ni(OH)_2$, is a candidate heat storage material. The mixed hydroxide was dehydrated, that is, it was capable of storing heats at 200–300 °C, at which pure $Mg(OH)_2$ could not be dehydrated and could not store heat. The heat output performance of the material was examined in a packed bed reactor. It was shown that the mixed hydroxide material was potentially useful for chemically storing medium-temperature heat such as waste heats emitted from internal combustion engines, solar energy system and high-temperature processes.

10/00289 The application of field synergy number in shell-and-tube heat exchanger optimization design

Guo, J. *et al. Applied Energy*, 2009, 86, (10), 2079–2087.

In the present work the field synergy principle is applied to the optimization design of the shell-and-tube heat exchanger with segmental baffles. The field synergy number which is defined as the indicator of the synergy between the velocity field and the heat flow is taken as the objective function. The genetic algorithm is employed to solve the heat exchanger optimization problems with multiple design variables. The field synergy number maximization approach for heat exchanger optimization design is thus formulated. In comparison with the initial design, the optimal design leads to a significant cost cut on the one hand and an improvement of the heat exchanger performance on the other hand. The comparison with the traditional heat exchanger optimization design approach with the total cost as the objective function shows that the field synergy number maximization approach is more advantageous.

10/00290 Theoretical analysis of a CO_2–NH_3 cascade refrigeration system for cooling applications at low temperatures

Dopazo, J. A. *et al. Applied Thermal Engineering*, 2009, 29, (8–9), 1577–1583.

As a result of environmental problems related to global warming and depletion of the ozone layer caused by the use of synthetic refrigerants (CFC's, HCFC's and HFC's) experienced over the last decades, the return to the use of natural substances for refrigeration purposes, appears to be the best long-term alternative. In this paper, a cascade refrigeration system with CO_2 and NH_3 as working fluids in the low and high temperature stages, respectively, has been analysed. Results of COP and exergetic efficiency versus operating and design parameters have been obtained. In addition, an optimization study based on the optimum CO_2 condensing temperature has been done. Results show that following both method's exergy analysis and energy optimization, an optimum value of condensing CO_2 temperature is obtained. The compressor isentropic efficiency influence on the optimum system COP has been demonstrated. A methodology to obtain relevant diagrams and correlations to serve as a guideline for design and optimization of this type of systems has been developed and it is presented in the paper.

10/00291 Thermal comfort enhancement by using a ceiling fan

Ho, H. S. *et al. Applied Thermal Engineering*, 2009, 29, (8–9), 1648–1656.

A parametric analysis on the effect of using a ceiling fan in an air-conditioned room is performed by two-dimensional (2D) numerical simulation of steady state airflow and heat transfer. Thermal comfort analysis is done for a person standing in a room with an inlet and an outlet for air conditioning and a ceiling fan. Representative three-dimensional (3D) simulation is also performed for the comparison of results obtained by using 2D and 3D models. Distributions of velocity, temperature, and relative humidity are presented. Different cases in which the ceilings fan may be not in use or in use with different air speed normal to the plane of fan blades due to different rotational speeds are considered. Predicted mean vote is computed and used to assess the thermal comfort characteristics. It is found that as the normal air speed from the fan increases, thermal comfort significantly shifts toward the cooler scale to allow higher supply air temperature or higher heat load in the room while maintaining the same comfort level.

10/00292 Thermal performance and embodied energy analysis of a passive house – case study of vault roof mud-house in India

Chel, A. and Tiwari, G. N. *Applied Energy*, 2009, 86, (10), 1956–1969.

This paper investigates thermal performance of an existing eco-friendly and low embodied energy vault roof passive house (or mud-house) located at Solar Energy Park of IIT Delhi, New Delhi (India). Based on embodied energy analysis, the energy payback time for the mud-house was determined as 18 years. The embodied energy per unit floor area of R.C.C. building (3702.3 MJ/m^2) is quiet high as compared to the mud-house (2298.8 MJ/m^2). The mud-house has three rooms with inverted U-shape roof and remaining three rooms with dome shape roof. A thermal model of the house consisting of six interconnected rooms was developed based on energy balance equations which were solved by using fourth order Runge Kutta numerical method. The predicted six room air temperatures were found in good agreement with the experimental observed data on hourly basis in each month for one year. The annual heating and cooling energy saving potential of the mud-house was determined as 1481 kW h/year and 1813 kW h/year respectively for New Delhi composite climate. The total mitigation of CO_2 emissions due to both heating and cooling energy saving potential was determined as 5.2 metric tons/year. The annual carbon credit potential of mud-house was determined as €52/year. Similar results were obtained for the different climatic locations in India.

10/00293 Thermal response of ground for different depths on vertical ground source heat pump system in Elaziğ, Turkey

Esen, H. and Inalli, M. *Journal of the Energy Institute*, 2009, 82, (2), 95–101.

The purpose of this study is to evaluate a heat pump system performance using the ground as a source and a sink of heat. The vertical ground source heat pump (VGSHP) system has three single U-tube ground heat exchangers (GHEs) made of polyethylene pipe with a 40 mm outside diameter. The GHEs were placed in a vertical borehole (VB) with depths of 30 m (VB1), 60 m (VB2) and 90 m (VB3) and 150 mm diameters. The experimental results were obtained in cooling and heating seasons of 2006–2007. The monthly mean values of coefficient of performance for VB1, VB2 and VB3 states are obtained to be 3.37/1.93, 3.85/2.37 and 4.33/3.03 respectively in cooling/heating modes. The coefficient of performance increases with increasing the borehole depths of VGSHP system. The energy efficiency and exergetic efficiencies of the system components are determined. Results obtained from experimental measurement concluded that the VGSHP systems can be used for Elaziğ, Turkey climatic conditions.

10/00294 Unsteady numerical simulation of the cooling process of vertical storage tanks under laminar natural convection

Rodríguez, I. *et al. International Journal of Thermal Sciences*, 2009, 48, (4), 708–721.

The transient cooling of a fluid initially at rest inside a vertical cylinder submitted to heat losses through the walls is studied. The study is restricted to laminar flow conditions. In order to identify the relevant non-dimensional groups that define the unsteady natural convection phenomenon that occurs, a non-dimensional analysis is carried out. The long-term behaviour of the fluid is modelled by formulating a prediction model based on global balances. A parametric study by means of several multidimensional numerical simulations led to correlate the Nusselt number and the transient mean fluid temperature, in order to feed the global model proposed. Special attention is given to the appropriateness of the spatial and time discretization adopted, the verification of the numerical solutions and the post-processing tasks carried out in order to obtain the correlations. The most relevant particularities of the numerical model developed are also pointed out.

10/00295 Variations in gas properties in laminar micro-convection with entrance effect

Gulhane, N. P. and Mahulikar, S. P. *International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1980–1990.

The present work investigates the influence of property variations of air in laminar forced convection with entrance effect. Two-dimensional micro-sized geometry (with axisymmetry) with constant wall heat flux boundary condition is considered to predict flow behaviour and thermal development. The continuum-based conservation equations are numerically solved to account for non-rarefaction scaling effects due to variations in fluid properties. At the microscale, results for Nusselt number show significant deviation from conventional theory that does not consider additional mechanisms that surface. The effect of property variation in Graetz problem for low subsonic flow is also studied.

11 ENGINES

Power generation and propulsion, electrical vehicles

10/00296 Chemical mechanism for high temperature combustion of engine relevant fuels with emphasis on soot precursors

Blanquart, G. *et al. Combustion and Flame*, 2009, 156, (3), 588–607.

This article presents a chemical mechanism for the high temperature combustion of a wide range of hydrocarbon fuels ranging from methane to iso-octane. The emphasis is placed on developing an accurate model for the formation of soot precursors for realistic fuel surrogates for premixed and diffusion flames. Species like acetylene (C_2H_2), propyne (C_3H_4), propene (C_3H_6), and butadiene (C_4H_6) play a major role in the formation of soot as their decomposition leads to the production of radicals involved in the formation of polycyclic aromatic hydrocarbons (PAH) and the further growth of soot particles. A chemical kinetic mechanism is developed to represent the combustion of these molecules and is validated against a series of experimental data sets including laminar burning velocities and ignition delay times. To correctly predict the formation of soot precursors from the combustion of engine relevant fuels, additional species should be considered. One normal alkane (*n*-heptane), one ramified alkane (iso-octane), and two aromatics (benzene and toluene) were chosen as chemical species representative of the components typically found in these fuels. A sub-mechanism for the combustion of these four species has been added, and the full mechanism has been further validated. Finally, the mechanism is supplemented with a sub-mechanism for the formation of larger PAH molecules up to cyclo[cd]pyrene. Laminar premixed and counterflow diffusion flames are simulated to assess the ability of the mechanism to predict the formation of soot precursors in flames. The final mechanism contains 149 species and 1651 reactions (forward and backward reactions counted separately). The mechanism is available with thermodynamic and transport properties as supplemental material.

10/00297 Effect of hydrogen addition on the idle performance of a spark ignited gasoline engine at stoichiometric condition

Ji, C. and Wang, S. *International Journal of Hydrogen Energy*, 2009, 34, (8), 3546–3556.

With regard to the improvement of efficiency, combustion stability, and emissions in a gasoline engine at idle condition, an experimental study aimed at improving engine idle performance through hydrogen addition was carried out on a four-cylinder gasoline-fueled spark ignited (SI) engine. The engine was modified to be fueled with the mixture of gasoline and hydrogen injected into the intake ports simultaneously. A self-developed electronic control unit (DECU) was dedicatedly used to control the injection timings and injection durations of gasoline and hydrogen. Other parameters, such as spark timing and idle valve opening, were controlled by the original engine electronic control unit (OECU). Various hydrogen enrichment levels were selected to investigate the effect of hydrogen addition on engine speed fluctuation, thermal efficiency, combustion characteristics, cyclic variation and emissions under idle and stoichiometric conditions. The experimental results showed that thermal efficiency, combustion performance, NO_x emissions are improved with the increase of hydrogen addition level. The HC and CO emissions first decrease with the increasing hydrogen enrichment level, but when hydrogen energy fraction exceeds 14.44%, it begins to increase again at idle and stoichiometric conditions.

10/00298 Heat transfer model for small-scale spark-ignition engines

Wu, Y.-Y. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1875–1886.

A heat transfer model for small-scale spark-ignition engines has been proposed by authors in previous study. However, that model was developed based on experimental data of one engine, it may not be so accurate for others. In order to improve the accuracy of predicted heat transfer rate for different engines, a modified heat transfer model using Stanton number based on two engines is proposed. Prediction results of instantaneous heat flux, global heat transfer, heat release rate, and cylinder pressure based on the proposed model are compared with the experimental results of three engines and prediction results of previous model. It is found that the proposed model has prediction results closer to the measured data than the previous models at the most engine operation conditions.

10/00299 Shaker-based heat and mass transfer in liquid metal cooled engine valves

Sander, W. and Weigand, B. *International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2552–2564.

The highly transient process of the working combustion engine generates a ‘shaker-effect’ inside the hollow valve stem where liquid sodium carries the heat from the hot valve head to the valve stem. Here it can pass through the valve guide, based on convective heat transfer and thermal conduction. The efficiency of these transport mechanisms is still not clearly understood, since the design of many liquid cooled valves is mostly based on empirical knowledge and can lead under certain conditions to a breakdown of the system. A simulation of the processes during the movement of the valve including detailed insight into the highly transient and complex two-phase flow phenomena as well as the heat transfer has been realized by means of direct numerical simulation (DNS) based on the volume-of-fluid (VOF) method. The influence of several relevant influencing factors such as the geometry, the acceleration and the liquid fill level were studied. It was found that the fill level is one of the most influencing factors regarding the efficiency of the heat transfer whereas the influence of geometrical dimensions and in particular the aspect ratio of the cavity were almost negligible in this setup. By averaging the fluid flow and the temperature field it has been shown that liquid cooled valves are more efficient compared to a solid valve but clustering of the liquid filling can appear which causes a temporal breakdown of the ‘shaker-effect’. In addition the influence of the spatial resolution is shown and 2D vs 3D simulation setups are compared. To the authors’ knowledge, no similar heat transfer predictions of the presented type are published in the literature.

10/00300 Study of the performance, emission and combustion characteristics of a diesel engine using poon oil-based fuels

Devan, P. K. and Mahalakshmi, N. V. *Fuel Processing Technology*, 2009, 90, (4), 513–519.

Experiments were conducted to study the performance, emission and combustion characteristics of a DI diesel engine using poon oil-based fuels. In the present work, poon oil and poon oil methyl ester are tested as diesel fuels in Neat and blended forms. The blends were prepared with 20% poon oil and 40% poon oil methyl ester separately with standard diesel on a volume basis. The reductions in smoke, hydrocarbon and carbon monoxide emissions were observed for poon oil methyl ester and its diesel blend along with increased NO_x emission compared to those of standard diesel. However, a reduction in NO_x emission and an increase in smoke, hydrocarbon and CO emissions were observed for Neat poon oil and its diesel blend compared to those of standard diesel. The 40% poon oil methyl ester blend showed a 2% increase in brake thermal efficiency compared to that of standard diesel, whereas other fuels tested showed a decreasing trend. From the combustion analysis it was found that ignition delay was shorter for all fuels tested compared to that of standard diesel. The combustion characteristics of poon oil methyl ester and its diesel blend closely followed those of standard diesel.

10/00301 Visualization of auto-ignition and pressure wave during knocking in a hydrogen spark-ignition engine

Kawahara, N. and Tomita, E. *International Journal of Hydrogen Energy*, 2009, 34, (7), 3156–3163.

Visualizations of auto-ignition inside the end-gas region due to flame propagation and pressure waves that occur during knocking were carried out in a hydrogen spark-ignition engine using a high-speed camera. These results demonstrated that auto-ignition in an end-gas region that was compressed by the propagating flame front could be visualized using the high-speed color camera. A large amount of unburned mixture caused by the auto-ignited kernel explosion generated the strong pressure waves. Strong pressure wave oscillations induced by the initial auto-ignition could be visualized using a video camera with a speed of 250 kframes/s. The auto-ignition and pressure waves caused the thermal boundary layer to breakdown near the cylinder wall and piston head, therefore combustion of the lubricant oil grease was visible inside burned gas region. This auto-ignition and pressure waves may result in damage to the cylinder wall and piston head during engine knocking.

Transport battery development

10/00302 Battery energy storage technology for power systems – an overview

Divya, K. C. and Østergaard, J. *Electric Power Systems Research*, 2009, 79, (4), 511–520.

The penetration of renewable sources (particularly wind power) in to the power system network has been increasing in the recent years. As a result of this, there have been serious concerns over reliable and satisfactory operation of the power systems. One of the solutions being proposed to improve the reliability and performance of these systems is to integrate energy storage devices into the power system network. Further, in the present deregulated markets these storage devices could also be used to increase the profit margins of wind farm owners and even provide arbitrage. This paper discusses the present status of battery energy storage technology and methods of assessing their economic viability and impact on power system operation. Further, a discussion on the role of battery storage systems of electric hybrid vehicles in power system storage technologies had been made. Finally, the paper suggests a likely future outlook for the battery technologies and the electric hybrid vehicles in the context of power system applications.

10/00303 Diesel fuel reformer for automotive fuel cell applications

Lindström, B. *et al. International Journal of Hydrogen Energy*, 2009, 34, (8), 3367–3381.

This paper describes an innovative and environmentally benign hydrogen generation system operating on commercial diesel fuel to avoid running the engine to supply electricity at stand-still. The use of a fuel cell-based auxiliary power unit (APU) has the potential of delivering electricity at high efficiencies independent of the heavy-duty truck engine. During the reformer development phase, spray formation and mixing of reactants proved to be crucial to obtain high reforming efficiencies and low diesel slip. The diesel is being injected through a nozzle creating a spray of fine droplets of a size which can establish rapid evaporation. Air and steam are being pre-heated and injected into the mixture chamber and subsequently mixed with the evaporated diesel fuel. Depending on the operating parameters, a part of the fuel is being oxidized and produces heat. Autothermal reforming was chosen to circumvent the heat transfer problem in catalytic steam reforming. By supplying heat directly to the catalyst surface by an oxidation reaction the heat demand of the strongly endothermic steam reforming reaction can be fulfilled. CFD calculations were employed that revealed the importance of avoiding large recirculation zones leading to a prolonged residence time of the hydrocarbon molecules and causing auto-ignition and excessive temperatures in the catalyst. Five different reformer generations are being described and discussed in detail in this publication. The first one was based on a fixed bed reactor, while the other four all relied on catalytic monoliths enabling low pressure drops. The early reactor designs all suffered from auto-ignition and instability problems. The latter generations exhibited a considerably more stable temperature profile in the reformer. The conversion of diesel and the reformer efficiencies are significantly higher than the early generation diesel reformers.

10/00304 First principles computational materials design for energy storage materials in lithium ion batteries

Meng, Y. S. and Arroyo-de Dompablo, M. E. *Energy Environmental Science*, 2009, 2, (6), 589–609.

First principles computation methods play an important role in developing and optimizing new energy storage and conversion materials. This review presents an overview of the computation approach aimed at designing better electrode materials for lithium ion batteries. Specifically, the authors show how each relevant property can be related to the structural component in the material and can be computed from first principles. By direct comparison with experimental observations, it is hoped to illustrate that first principles computation can help to accelerate the design and development of new energy storage materials.

10/00305 Hybrid fuel cell-based energy system with metal hydride hydrogen storage for small mobile applications

Guizzi, G. L. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 3112–3124.

This paper describes the general architecture of a hybrid energy system, whose main components are a proton exchange membrane fuel cell, a battery pack and an ultracapacitor pack as power sources, and metal hydride canisters as energy storage devices, suitable for supplying power to small mobile non-automotive devices in a flexible and variable way. The first experimental results carried out on a system prototype are described, showing that the extra components, required in order to manage the hybrid system, do not remarkably affect the overall system efficiency, which is always higher than 36% in all the test configurations examined. In fact, the system allows the fuel cell to work most often at quasi-optimal conditions, near its maximum efficiency (i.e. at low/medium loads), because high external loads are met by the combined effort of the fuel cell and the ultracapacitors. For the same reason, the metal hydride storage system can be used also under highly dynamic operating conditions, notwithstanding its usually poor kinetic performance.

10/00306 Integration of methanol steam reforming and combustion in a microchannel reactor for H_2 production: a CFD simulation study

Arzamendi, G. *et al. Catalysis Today*, 2009, 143, (1–2), 25–31.

A computational fluid dynamics (CFD) study of the thermal integration of the steam reforming of methanol (SRM) and the combustion of methanol in a catalytic microchannel reactor is presented. This issue is of interest for *in situ* H_2 production for portable power units based on low-temperature PEM fuel cells. Three-dimensional simulations have been carried out under relevant conditions for the SRM reaction that have shown that microreactors allow complete methanol reforming and combustion at space velocities as high as $50{,}000\,h^{-1}$, with selectivities for H_2 above 99% at relatively low temperatures in the 270–290 °C range.

10/00307 Novel surface treatment for hydrogen storage alloy in Ni/MH battery

Zhao, X. *et al. International Journal of Hydrogen Energy*, 2009, 34, (8), 3506–3510.

A novel surface treatment for the $MlNi_{3.8}Co_{0.75}Mn_{0.4}Al_{0.2}$ (La-rich mischmetal) hydrogen storage alloy has been carried out by using an aqueous solution of HF and KF with a little addition of KBH_4. The results of scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS) showed that rough surface was formed and Al was partly dissolved into the solution after the treatment. The result of XPS indicated the formation of Ni_3B and LaF_3 compounds on the alloy surface by the treatment. The probable chemical reaction mechanism for the surface treatment was introduced. The treatment resulted in significant improvements in the activation property, discharge capacity and cycle life of the alloy, especially the high rate dischargeability (HRD). The HRD of the treated alloy still remained 54.9% while that of the untreated one was only 15.1% at a discharge current density of 1200 mA/g.

10/00308 Ten-year efforts and a no-go recommendation for sodium borohydride for on-board automotive hydrogen storage

Demirci, U. B. *et al. International Journal of Hydrogen Energy*, 2009, 34, (6), 2638–2645.

In the early 2000s, sodium borohydride ($NaBH_4$) was presented as a promising hydrogen storage material with an ideal gravimetric hydrogen storage capacity of 10.8 wt%. Despite 10-year efforts in research and development, the US Department of Energy (US DOE) recommended a no-go for $NaBH_4$ for on-board automotive hydrogen storage. The US DOE decision was based on the following observations: too low effective gravimetric hydrogen storage capacities, inefficiency of hydrolysis by-product ($NaBO_2$) recycling, and cost. The present paper illustrates this decision using state-of-the-art open international literature. Furthermore as the decision clearly focuses on automotive applications, the authors attempt to show that $NaBH_4$ may have a potential for portable applications.

12 REFRACTORIES/ CERAMICS

Properties, production, applications

10/00309 Electrically switchable chromogenic materials for external glazing

Cupelli, D. *et al. Solar Energy Materials and Solar Cells*, 2009, 93, (3), 329–333.

The development of chromogenic materials is important for their potential applications as electrically adjustable or thermally self-adjusting light and heat filters in the external glazing of buildings. Recently, the authors have reported their investigations on electrolyte–liquid crystal dispersions, which show independent electro-optical and electrochromic properties characterized by fast bleaching times. Nevertheless, for the external glazing of buildings, it is recommended to have a transparent off state, which turns opaque upon application of the external field. This paper presents efforts to homeotropically align by rough surfaces fluid mixtures of a low molecular mass liquid crystal with a negative dielectric anisotropy, a liquid crystalline monomer, and electrolyte molecules in order to obtain transparent films after a polymerization process. Upon application of an ac electric field, the device becomes opaque and if a dc field is added, the cell changes colour too. The study also investigated the relationship between electro-optical/chromogenic response and physical chemical properties of the components.

10/00310 Formation and optical properties of copper nanoclusters in a silicate glass

Zhang, J. and Sheng, J. *International Journal of Hydrogen Energy*, 2009, 34, (8), 3531–3534.

In this letter, copper nanoclusters formation was observed in Cu-doped silicate glasses after UV-light irradiation followed by thermal annealing. After heating at 460 °C for 45 min, the Cu nanoclusters formed only in the UV-light irradiated glass, but not appeared in the un-irradiated sample. The critical temperature around at 460 °C was found in the irradiated sample to form Cu nanoclusters. Thermal annealing at the temperature above this critical point would form Cu nanoclusters both in the irradiated and un-irradiated glasses. Compared to the un-irradiated sample, the UV-light irradiated glass usually had more free electrons, and then more Cu^+ could trap electrons to form atoms.

10/00311 High-efficiency multistable switchable glazing using smectic A liquid crystals

Gardiner, D. J. *et al. Solar Energy Materials and Solar Cells*, 2009, 93, (3), 301–306.

Presently, nematic polymer dispersed liquid crystals (PDLCs) that are used in switchable glazing technology require constant power to operate and, moreover, exhibit unwanted haze at wide viewing angles. In this paper, a novel switchable glazing technology, based around a bistable electro-optic effect in the Smectic A liquid crystal phase, is described which does not require constant power to operate or exhibit haze. The application of a low-frequency (100 Hz) voltage induces an optically opaque state due to the motion of ionic material whereas the application of a higher frequency AC (1 kHz) voltage induces a haze-free clear state. Multistable (greyscale) operation is possible through the application of intermediate frequencies or voltages; the threshold voltages of the effect were found to range from 36 to 66 V rms. Any voltage-induced state is preserved indefinitely after removal of the voltage leading to low power consumption.

10/00312 Hydrodynamic and mass transfer efficiency of ceramic foam packing applied to distillation

Lévêque, J. *et al. Chemical Engineering Science*, 2009, 64, (11), 2607–2616.

In addition to a high void volume and specific area, solid foams possess other properties (low density, good thermal, mechanical, electrical, and acoustical behaviour) that make them attractive for applications such as heat exchangers and reformers. Applications using foams as catalysts or structured catalyst supports have demonstrated higher performance than classical catalysts. Several studies have explored the hydrodynamic behaviour of foams in monophasic and countercurrent systems and have reported very low pressure drops. This paper describes the application of ceramic foam to distillation. The β-SiC foam contains 5 pores per inch (PPI) with a 91% void volume and a surface area of $640\,m^2/m^3$. Performance parameters including pressure drop for the dry and wet packing, flooding behaviour, and dynamic liquid hold-up were measured in a column of 150 mm internal diameter. The mass transfer efficiency in terms of the height equivalent to theoretical plate (HETP) was determined by total reflux experiments using a mixture of *n*-heptane and cyclohexane at atmospheric pressure. The experimental results were used to develop a set of correlations describing pressure drop and liquid hold-up in terms of a dimensionless number. The hydrodynamic performance and mass transfer efficiency were compared with classical packing materials used in distillation.

10/00313 KrF-excimer laser irradiation on the soda-lime silicate glass

Zhang, J. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 3197–3200.

Defects induced by KrF-excimer laser irradiation in the soda-lime silicate glass were studied by means of optical spectrophotometric and electron spin resonance measurements. Three induced absorption bands at peak position of 610, 420, and 275 nm were determined in the glass after the UV-laser radiation, with the assistance of Gaussian resolution method. The defects of non-bridging oxygen hole centers attributed to two absorption peaks at 610 and 420 nm, and the trapped electrons correlated to the absorption at 275 nm. The induced absorption bands increased when laser irradiation time or energy density increased.

10/00314 Temperature amplification during laser heating of polycrystalline silicon microcantilevers due to temperature-dependent optical properties

Serrano, J. R. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (9–10), 2255–2264.

The absorption of optical energy and subsequent thermal transport are investigated experimentally and numerically for 500 μm long, 250 μm wide, and 2.25 μm thick polycrystalline silicon microcantilevers irradiated by an 808 nm continuous-wave laser. Temperature profiles were measured using Raman thermometry at 314 and 532 mW of laser power, and the microcantilever peak temperature was measured for laser powers up to 719 mW. A modular technique for multilayered structures is used to calculate the optical absorption in polysilicon microcantilevers, and the thermal response is then calculated with a two-dimensional, finite difference model. Very good agreement is obtained between the measured and calculated temperature profiles and peak temperatures versus laser power. The abrupt increase or amplification of peak temperature for laser powers between 415 and 440 mW is shown to be a result of peaks in the temperature-dependent optical absorptance.

10/00315 Well-aligned single-crystalline silicon nanowire hybrid solar cells on glass

Huang, J.-S. *et al. Solar Energy Materials and Solar Cells*, 2009, 93, (5), 621–624.

Hybrid solar cells are fabricated on the glass substrate using well-aligned single-crystalline Si nanowires (SiNWs) and poly(3-hexylthiophene):[6,6]-phenyl-C_{61}-butyric acid methyl ester (P3HT:PCBM). Their key benefits are discussed. The well-aligned SiNWs are fabricated from Si wafer and transferred onto the glass substrate with the P3HT:PCBM. Such SiNWs provide uninterrupted conduction paths for electron transport, enhance the optical absorption to serve as an interesting candidate of the absorber, and increase the surface area for exciton dissociation. These investigations show that SiNWs are promising for hybrid organic photovoltaic cells with improved performance by increasing the short-circuit current density from 7.17 to $11.61\,mA/cm^2$.

13 ALTERNATIVE ENERGY SUPPLIES

Biofuels and bioconversion energy

10/00316 An ablation model for the thermal decomposition of porous zinc oxide layer heated by concentrated solar radiation

Dombrovsky, L. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2444–2452.

Thermal decomposition of porous ZnO under high-flux solar irradiation is considered. The process is well described by a transient ablation model that couples radiation, conduction, and convection heat transfer to an Arrhenius-type kinetic rate law with a pre-exponential factor dependent on the porosity, grain/pore size, and convective removal of the reaction products Zn(g) and O_2. Main model parameters are determined by comparing numerical and experimental results.

10/00317 An approach to calculate solid–liquid phase equilibrium for binary mixtures

Rocha, S. A. and Guirardello, R. *Fluid Phase Equilibria*, 2009, 281, (1), 12–21.

An approach is presented to calculate solid–liquid phase equilibrium for binary mixtures, using expressions for the temperature as a function of the molar fraction. For Margules model the expression gives explicitly the temperature, while for other liquid phase activity models an iterative procedure is required to calculate the temperature. The method is very easy to apply and it can be used for mixtures that have peritectic and eutectic points, or just a eutectic point. The approach was applied to five case studies with binary mixtures of fatty acids and triglycerides. The results were in good agreement with experimental data.

10/00318 Application of CFD to model fast pyrolysis of biomass

Papadikis, K. *et al. Fuel Processing Technology*, 2009, 90, (4), 504–512.

The article deals with the CFD modelling of fast pyrolysis of biomass in an entrained flow reactor (EFR). The Lagrangian approach is adopted for the particle tracking, while the flow of the inert gas is treated with the standard Eulerian method for gases. The model includes the thermal degradation of biomass to char with simultaneous evolution of gases and tars from a discrete biomass particle. The chemical reactions are represented using a two-stage, semi-global model. The radial distribution of the pyrolysis products is predicted as well as their effect on the particle properties. The convective heat transfer to the surface of the particle is computed using the Ranz–Marshall correlation.

10/00319 Beef tallow biodiesel produced in a pilot scale

da Cunha, M. E. *et al. Fuel Processing Technology*, 2009, 90, (4), 570–575.

In the present work, the process of biodiesel production in a pilot plant has been studied using beef tallow as raw materials with methanol and potassium hydroxide as catalyst. The biodiesel quality is regulated by Brazilian specifications (Resolution 42) by the National Agency of Petroleum (ANP). The alkaline transesterification of animal fat with methanol produces a biodiesel of high quality and also with a good conversion rate. The process is possible but the economical viability must be improved by recovering methanol and glycerin. The obtained results have been used for industrial scale-up of the process.

10/00320 Biodiesel preparation using Li/CaO catalysts: activation process and homogeneous contribution

Alonso, D. M. *et al. Catalysis Today*, 2009, 143, (1–2), 167–171.

This work studies the influence of the lithium content and activation temperature of Li-doped CaO catalysts in the transesterification reaction of triglycerides with methanol and the homogeneous contribution. Several samples with different lithium content have been studied, and a lithium concentration >3.6 wt% of lithium was expected to exert a promoter effect. The influence of activation temperature has been investigated for 4.5LiCa catalyst, requiring a temperature of activation above the melting point of $LiNO_3$ (492 K) to observe any catalytic activity. Moreover, it has been observed that the homogeneous contribution, and consequently the amount of lithium species leached, depends on activation temperature: the leaching of lithium and homogeneous contribution is significant for activation temperatures $\geq$973 K (87% in 3 h), when Li oxides was present in the sample, whereas the homogeneous contribution is little relevant at activation temperatures $\leq$773 K, where $LiNO_3$ has not yet decomposed. Consequently at activation temperatures between 773 and 973 K, an intermediate situation, will be expected.

10/00321 Biohydrogen production from wastewater by *Clostridium beijerinckii*: Effect of pH and substrate concentration

Skonieczny, M. T. and Yargeau, V. *International Journal of Hydrogen Energy*, 2009, 34, (8), 3288–3294.

An investigation of biological hydrogen production from glucose by *Clostridium beijerinckii* was conducted in a synthetic wastewater solution. A study examining the effect of initial pH (range 5.7–6.5) and substrate loading (range 1–3 g COD/L) on the specific conversion and hydrogen production rate has shown interaction behaviour between the two independent variables. Highest conversion of 10.3 mL H_2/(g COD/L) was achieved at pH of 6.1 and glucose concentration of 3 g COD/L, whereas the highest production rate of 71 mL H_2/(h L) was measured at pH 6.3 and substrate loading of 2.5 g COD/L. In general, there appears to be a strong trend of increasing hydrogen production rate with an increase in both substrate concentration and pH. Butyrate (14–63%), formate (10–45%) and ethanol (16–40%) were the main soluble products with other volatile fatty acids and alcohols present in smaller quantities.

10/00322 Co-processing of pyrolysis bio oils and gas oil for new generation of bio-fuels: hydrodeoxygenation of guaïacol and SRGO mixed feed

Bui, V. N. *et al. Catalysis Today*, 2009, 143, (1–2), 172–178.

Within the framework of second-generation bio-fuels development, the present work reports on the impact of co-processing guaiacol as an oxygenated molecule representative of pyrolitic bio-oils with a straight run gas oil (SRGO) in the framework of a hydrodesulfurization process (HDS). The reaction scheme observed during the hydrotreating of the sole guaiacol in the gas phase was compared to the conversion products observed during the co-processing of guaiacol with the SRGO, by using two-dimensional GC–MS analysis. During the co-processing, a decrease of the HDS performance of a reference $CoMo/Al_2O_3$ catalyst was observed at a low temperature and high contact time. It was assigned to the formation of intermediate phenols competing with sulfur containing molecules for adsorbing on hydrogenation/hydrogenolysis sites. Above 320 °C, complete hydrodeoxygenation (HDO) of guaiacol was observed and HDS could proceed without any further inhibition.

10/00323 Dark fermentation of ground wheat starch for bio-hydrogen production by fed-batch operation

Kargi, F. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 2940–2946.

Ground wheat solution was used for bio-hydrogen production by dark fermentation using heat-treated anaerobic sludge in a completely mixed fermenter operating in fed-batch mode. The feed wheat powder (WP) solution was fed to the anaerobic fermenter with a constant flow rate of $8.33\,mL\,h^{-1}$ ($200\,mL\,d^{-1}$). Cumulative hydrogen production, starch utilization and hydrogen yields were determined at three different WP loading rates corresponding to the feed WP concentrations of 10, 20 and $30\,g\,L^{-1}$. The residual starch (substrate) concentration in the fermenter decreased with operation time while starch consumption was increasing. The highest cumulative hydrogen production (3600 mL), hydrogen yield ($465\,mL\,H_2\,g^{-1}$ starch or 3.1 mol $H_2\,mol^{-1}$ glucose) and hydrogen production rate ($864\,mL\,H_2\,d^{-1}$) were obtained after 4 days of fed-batch operation with the $20\,g\,L^{-1}$ feed WP concentration corresponding to a WP loading rate of $4\,g\,WP\,d^{-1}$. Low feed WP concentrations ($10\,g\,L^{-1}$) resulted in low hydrogen yields and rates due to substrate limitations. High feed WP concentrations ($30\,g\,L^{-1}$) resulted in the formation of volatile fatty acids (VFAs) in high concentrations causing inhibition on the rate and yield of hydrogen production.

10/00324 Design of solid catalysts for the conversion of biomass

Rinaldi, R. and Schüth, F. *Energy Environmental Science*, 2009, 2, (6), 610–626.

The discovery and investigation of novel and efficient pathways for the conversion of biomass into fuels and chemicals are among the big challenges facing heterogeneous catalysis nowadays. However, not all experience gained in the transformation of hydrocarbons over the last 100 years can directly be transferred to biomass conversion. The authors discuss how the specific properties of biomass pose new requirements on the processes and on the solids that are used as catalysts for their conversion. Due to the importance of lignocellulosic materials, which constitute about 95% of the total plant biomass, this paper will focus mostly on the desired properties of solid catalysts for the conversion of these polymeric biomolecules. Research in this field is very intense presently and novel transformations and catalysts are being discovered at a high rate. This study thus focuses on the concepts that govern biomass transformation instead of giving a complete and comprehensive survey of the literature, which would be outdated within a short time.

10/00325 Effects of temperature and substrate concentration on biological hydrogen production from starch

Akutsu, Y. *et al. International Journal of Hydrogen Energy*, 2009, 34, (6), 2558–2566.

This study investigates the effects of temperature and substrate concentration on biological hydrogen production from starch using mixed cultures. In this work, although hydrogen was successfully produced under the thermophilic condition, stable hydrogen production was not observed under the mesophilic condition. In the thermophilic reactor, the maximum hydrogen yield was 2.8 mol H_2/mol glucose at 20 g/l-starch; however, hydrogen yield decreased drastically with the change of by-product distribution when substrate concentration was over 30 g/l-starch. A negative correlation was observed between the hydrogen yield and the total concentration of undissociated acids.

10/00326 Effects of temperature at different organic loading levels on the performance of a fluidized-bed anaerobic sequencing batch bioreactor

Bergamo, C. M. *et al. Chemical Engineering and Processing: Process Intensification*, 2009, 48, (3), 789–796.

An investigation was performed on the effect of temperature and organic load on the stability and efficiency of a 1.8-L fluidized-bed anaerobic sequencing batch reactor (ASBR), containing granulated biomass. Assays were carried out employing superficial up flow velocity of 7 m/h, total cycle length of 6 h and synthetic wastewater volume of 1.3 L per cycle. The fluidized-bed ASBR was operated at 15, 20, 25 and 30 °C with influent organic matter concentrations of 500 and 1000 mgCOD/L. The system showed stability under all conditions and presented filtered samples removal efficiency ranging from 79 to 86%. A first-order kinetic model could be fitted to the experimental values of the organic matter concentration profiles. The specific kinetic parameter values of this model ranged from 0.0435 to 0.2360 L/(gTVS h) at the implemented operation conditions. In addition, from the slope of an Arrhenius plot, the activation energy values were calculated to be 16,729 and 12,673 cal/mol for operation with 500 and 1000 mgCOD/L, respectively. These results show that treatment of synthetic wastewater, with concentration of 500 mgCOD/L, was more sensitive to temperature variations than treatment of the same residue with concentration of 1000 mgCOD/L. Comparing the activation energy value for operation at 500 mgCOD/L with the value obtained in an earlier study in an ASBBR treating the same wastewater at the same concentration, the value obtained in the fluidized-bed ASBR showed to be superior, indicating that treatment of synthetic wastewater in a reactor containing granulated biomass was more sensitive to temperature variations than the treatment using immobilized biomass.

10/00327 Experimental investigation on mixing and segregation behavior of biomass particle in fluidized bed

Zhang, Y. *et al. Chemical Engineering and Processing: Process Intensification*, 2009, 48, (3), 745–754.

The mixing and segregation behaviour of biomass particles have been investigated experimentally in fluidized bed made up of biomass–sand mixture with different biomass/sand ratios. The biomass is cylindrical-shape cotton stalk, and the sand belongs to the Geldart B category. The initial bed is thoroughly mixed and the gas superficial velocity varies to cover a wide range. The mixing and segregation behaviour are analysed in terms of flow patterns, solid concentration profile and mixing index. It is found that as the gas superficial velocity gradually increases, the bed undergoes local segregation, global segregation, local mixing, global mixing and re-segregation.

10/00328 Highly efficient procedure for the synthesis of biodiesel from soybean oil

Liang, X. *et al. Fuel Processing Technology*, 2009, 90, (5), 701–704.

A novel and efficient procedure has been developed for the synthesis of biodiesel from soybean oil and methanol. K_2CO_3 supported on MgO has been selected as the most efficient catalyst for the reaction with the yield of 99%. Operational simplicity, low cost of the catalyst used, high yields, short reaction time and reusability are the key features of this methodology.

10/00329 Improving biodiesel fuel properties by modifying fatty ester composition

Knothe, G. *Energy Environmental Science*, 2009, 2, (7), 759–766.

Biodiesel is an alternative to petroleum-derived diesel fuel composed of alkyl esters of vegetable oils, animal fats or other feedstocks such as used cooking oils. The fatty acid profile of biodiesel corresponds to that of its feedstock. Most common feedstocks possess fatty acid profiles consisting mainly of five C_{16} and C_{18} fatty acids, namely, palmitic (hexadecanoic), stearic (octadecanoic), oleic (9(*Z*)-octadecenoic), linoleic (9(*Z*),12(*Z*)-octadecadienoic) and linolenic (9(*Z*),12(*Z*),15(*Z*)-octadecatrienoic) acids, with the exception of a few oils such as coconut oil, which contains high amounts of saturated acids in the C_{12}–C_{16} range or others. While in many respects biodiesel possesses advantages or is competitive with petroleum-derived diesel fuel, virtually all biodiesel fuels, typically the methyl esters, produced from these oils have performance problems such as poor low-temperature properties or insufficient oxidative stability. Considerable research has focused on solving or alleviating these problems and five approaches have been developed. Besides the approach of using additives, changing the fatty ester composition by either varying the alcohol or the fatty acid profile of the oil have been studied. Changing the fatty acid profile can be achieved by physical means, genetic modification of the feedstock or use of alternative feedstocks with different fatty acid profiles. In some cases approaches may overlap. This article briefly summarizes the five approaches currently used with an emphasis on those dealing with changing the fatty ester composition of a biodiesel fuel.

10/00330 Investigation of gas properties, design, and operational parameters on hydrodynamic characteristics, mass transfer, and biomass production from natural gas in an external airlift loop bioreactor

Yazdian, F. *et al. Chemical Engineering Science*, 2009, 64, (10), 2455–2465.

An external airlift loop bioreactor (EALB) was used for production of biomass from natural gas. The effect of riser to downcomer cross-sectional area ratio (A_r/A_d), volume of gas–liquid separator, superficial gas velocity (U_{sgr}), and physical properties of gases and their mixtures [$\upsilon_g(\mu/\rho)$ and D_g] were investigated on mixing time, gas hold-up, and volumetric gas liquid mass transfer coefficients (k_La). It was found that A_r/A_d has remarkable effects on gas hold-up and k_La due to its influence on mixing time. Kinematic viscosity (υ_g) showed its significant role on mixing time, gas hold-up and k_La when different gases used (mixing time changes directly whereas gas hold-up and k_La change indirectly). Moreover, it was found that diffusion coefficient of gas in water (D_g) has remarkable effect on k_La. The volumetric mass transfer coefficients for methane and its mixtures with oxygen (three different mixtures) were determined at different geometrical and operational factors. In average, the rate of oxygen utilization is approximately 1.8 times higher than that of methane. A gas mixture of 25 vol% methane and 75 vol% oxygen was the best gas mixture for biomass production in the EALB. The correlations developed for predicting the mixing time, gas hold-up, and k_La in terms of U_{sgr}, A_r/A_d, volume of gas–liquid separator, and gas phase properties have been found to be encouraging.

10/00331 Kinetics of delignification using a batch reactor with recycle

Macfarlane, A. L. *et al. Chemical Engineering and Processing: Process Intensification*, 2009, 48, (4), 864–870.

Delignification kinetics for organosolv pulping of willow was determined using a novel method. Traditional methods of determining reaction rates and activation energy in pulping experiments involve analysis of the solid wood fraction for lignin content after pulping. This requires a large number of experimental runs to be performed to produce pulped wood having different final lignin content corresponding to different treatment time and temperature. In this paper, only four experiments are used in a reactor with a long heat up time and kinetic constant is determined at varying temperatures during the heat up period. This greatly reduces the number of runs required by obtaining many *k* values in only one run. The kinetics of organosolv delignification of hardwoods, namely *Salix schwerinii*, is determined and the activation energies obtained agree with previous work.

10/00332 Pretreatment and feeding of biomass for pressurized entrained flow gasification

Svoboda, K. *et al. Fuel Processing Technology*, 2009, 90, (5), 629–635.

This study compared the advantages and disadvantages of four different methods for biomass (wood) thermal pretreatment and grinding for feeding of biomass-fuel to the pressurized entrained flow gasifier. The four methods of pretreatment and feeding involve drying, torrefaction, flash pyrolysis and dissolution of wood in organic solvents. The resulting fuels after pretreatment are compared in terms of heating value, grinding energy needed, overall efficiency of conversion (from raw biomass to fuel), auxiliary energy needed, fluidization properties, pneumatic feeding properties, pumping, viscosity and possible changes of properties of liquids/slurry, storage, microbial attack, emissions from thermal pretreatment and overall integration with pressurized entrained flow gasification.

10/00333 Production of biodiesel from palm oil (*Elaeis guineensis*) using heterogeneous catalyst: an optimized process

Hameed, B. H. *et al. Fuel Processing Technology*, 2009, 90, (4), 606–610.

Response surface methodology (RSM) based on central composite design (CCD) was used to optimize the three important reaction variables – methanol/oil molar ratio (x_1), reaction time (x_2) and amount of catalyst (x_3) for production of biodiesel from palm oil using KF/ZnO catalyst. Based on the CCD, a quadratic model was developed to correlate the reaction variables to the biodiesel yield. From the analysis of variance (ANOVA), the most influential factor on the experimental design response was identified. The predicted yield after process optimization was found to agree satisfactory with the experimental value. The optimum conditions for biodiesel production were found as follows: methanol/oil ratio of 11.43, reaction time of 9.72 h and catalyst amount of 5.52 wt%. The optimum biodiesel yield was 89.23%.

10/00334 Separation of bio-oil by molecular distillation

Wang, S. *et al. Fuel Processing Technology*, 2009, 90, (5), 738–745.

In this study, KDL5 molecular distillation apparatus manufactured by the UIC Corporation was adopted to separate bio-oil, which came from a bench-scale fluidized-bed fast pyrolysis reactor at a feeding rate of

1 kg/h. A maximum distillate yield of 85% was obtained without obvious coking or polymerization during the molecular distillation process. The effect of distillation temperature on physical and chemical characterization of each bio-oil fraction was investigated. Statistical calculations showed that molecular distillation was successful in the separation of bio-oil. A separation factor was proposed to reflect the ability of isolating the chemicals contained in the bio-oil using molecular distillation.

10/00335 Solar hydrogen production by two-step thermochemical cycles: evaluation of the activity of commercial ferrites

Fresno, F. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 2918–2924.

This work reports on the evaluation of the activity of commercially available ferrites with different compositions, $NiFe_2O_4$, $Ni_{0.5}Zn_{0.5}Fe_2O_4$, $ZnFe_2O_4$, $Cu_{0.5}Zn_{0.5}Fe_2O_4$ and $CuFe_2O_4$, for hydrogen production by two-step thermochemical cycles, as a preliminary study for solar energy driven water splitting processes. The samples were acquired from Sigma–Aldrich, and are mainly composed of a spinel crystalline phase. The net hydrogen production after the first reduction–oxidation cycle decreases in the order $NiFe_2O_4 > Ni_{0.5}Zn_{0.5}Fe_2O_4 > ZnFe_2O_4 > Cu_{0.5}Zn_{0.5}Fe_2O_4 > CuFe_2O_4$, and so does the H_2/O_2 molar ratio, which is regarded as an indicator of potential cyclability. Considering these results, the nickel ferrite has been selected for longer term studies of thermochemical cycles. The results of four cycles with this ferrite show that the H_2/O_2 molar ratio of every two steps increases with the number of cycles, being the total amount stoichiometric regarding the water splitting reaction. The possible use of this nickel ferrite as a standard material for the comparison of results is proposed.

Geothermal energy

10/00336 Thermodynamic assessment of geothermal energy use in hydrogen production

Balta, M. T. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 2925–2939.

In this study, geothermal-based hydrogen production methods, and their technologies and application possibilities are discussed in detail. A high-temperature electrolysis (HTE) process coupled with and powered by a geothermal source is considered for a case study, and its thermodynamic analysis through energy and exergy is conducted for performance evaluation purposes. In this regard, overall energy and exergy efficiencies of the geothermal-based hydrogen production process for this HTE are found to be 87% and 86%, respectively.

Solar energy

10/00337 A metal-free black dye for panchromatic dye-sensitized solar cells

Tian, H. *et al. Energy Environmental Science*, 2009, 2, (6), 674–677.

A novel metal-free black dye was designed and synthesized for panchromatic dye-sensitized solar cells. Based on this dye, the broader incident photon-to-current conversion efficiency spectrum was obtained over the whole visible range extending into the near-IR region up to 920 nm.

10/00338 Carbon nanotubes for lithium ion batteries

Landi, B. J. *et al. Energy Environmental Science*, 2009, 2, (6), 638–654.

Lithium ion batteries are receiving considerable attention in applications, ranging from portable electronics to electric vehicles, due to their superior energy density over other rechargeable battery technologies. However, the societal demands for lighter, thinner, and higher capacity lithium ion batteries necessitate ongoing research for novel materials with improved properties over that of state-of-the-art. Such an effort requires a concerted development of both electrodes and electrolyte to improve battery capacity, cycle life, and charge–discharge rates while maintaining the highest degree of safety available. Carbon nanotubes (CNTs) are a candidate material for use in lithium ion batteries due to their unique set of electrochemical and mechanical properties. The incorporation of CNTs as a conductive additive at a lower weight loading than conventional carbons, like carbon black and graphite, presents a more effective strategy to establish an electrical percolation network. In addition, CNTs have the capability to be assembled into free-standing electrodes (absent of any binder or current collector) as an active lithium ion storage material or as a physical support for ultra high capacity anode materials like silicon or germanium. The measured reversible lithium ion capacities for CNT-based anodes can exceed 1000 $mAh\,g^{-1}$ depending on experimental factors, which is a 3× improvement over conventional graphite anodes. The major advantage from utilizing free-standing CNT anodes is the removal of the copper current collectors which can translate into an increase in specific energy density by more than 50% for the overall battery design. However, a developmental effort needs to overcome current research challenges including the first cycle charge loss and paper crystallinity for free-standing CNT electrodes. Efforts to utilize pre-lithiation methods and modification of the single wall carbon nanotube bundling are expected to increase the energy density of future CNT batteries. Other progress may be achieved using open-ended structures and enriched chiral fractions of semiconducting or metallic chiralities that are potentially able to improve capacity and electrical transport in CNT-based lithium ion batteries.

10/00339 Direct coupling of an electrolyser to a solar PV system for generating hydrogen

Clarke, R. E. *et al. International Journal of Hydrogen Energy*, 2009, 34, (6), 2531–2542.

This paper examines direct coupling of a polymer electrolyte membrane (PEM) electrolyser to a matched solar photovoltaic (PV) source for hydrogen generation and storage. Such direct coupling with minimum interfacing electronics would lead to substantial cost reduction and thereby enhance the economic viability of solar-hydrogen systems. The electrolyser is designed for fail-safe operation with multiple levels of safety and operational redundancy. A control system in the electrolyser unit provides for disconnection when required and for auto-start in the morning and auto shut-down at night, simultaneously addressing the goals of minimum energy loss and maximum safety. The PV system is a 2.4 kW array (20.4 m^2 total area) comprising 30, 12 V, 80 W, Solarex polycrystalline modules in a series–parallel configuration. The integrated system was operated for approximately 60 days over a 4-month period from September 2007 to January 2008 with many periods of unattended operation for multiple days, experiencing weather ranging from hot and sunny (above 40 °C) to cool and cloudy. The principle and practicality of direct coupling of a suitably matched PV array and PEM electrolyser have been successfully demonstrated. Details of electrolyser operation coupled to a PV array along with modelling work to match current–voltage characteristics of the electrolyser and PV system are described.

10/00340 Efficient electron transport in tetrapod-like ZnO metal-free dye-sensitized solar cells

Chiu, W.-H. *et al. Energy Environmental Science*, 2009, 2, (6), 694–698.

The tetrapod-like ZnO nanopowders are employed to construct an efficient electron transport network as the photoanode of the dye-sensitized solar cells (DSCs). Due to the high extinction coefficient of the metal-free D149 dye offering a high photocurrent through the ZnO network, the best performance of DSCs based on a 42 μm terapod-like ZnO film showed a high energy conversion efficiency of 4.9% with a high short-circuit photocurrent density of 12.3 $mA\,cm^{-2}$, an open-circuit photovoltage of 0.6 V, and a fill factor of 0.65 under AM 1.5 irradiation. Highly efficient electron transport may also be ascribed by a long effective electron diffusion length of 46 μm determined from the electrochemical impedance spectroscopy which is consistent with thickness dependent J_{SC} measurements.

10/00341 Exergy analysis of direct expansion solar-assisted heat pumps using artificial neural networks

Mohanraj, M. *et al. International Journal of Energy Research*, 2009, 33, (11), 1005–1020.

Artificial neural network (ANN) is applied for exergy analysis of a direct expansion solar-assisted heat pump (DXSAHP) in the present study. The experiments were conducted in a DXSAHP under the meteorological conditions of Calicut city in India. An ANN model was developed based on backpropagation learning algorithm for predicting the exergy destruction and exergy efficiency of each component of the system at different ambient conditions (ambient temperature and solar intensity). The experimental data acquired are used for training the network. The results showed that the network yields a maximum correlation coefficient with minimum coefficient of variance and root mean square values. The results confirmed that the use of an ANN analysis for the exergy evolution of DXSAHP is quite suitable.

10/00342 Experimental investigations on heat transfer and frictional characteristics of a turbulator roughened solar air heater duct

Bopche, S. B. and Tandale, M. S. *International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2834–2848.

An experimental investigation has been carried out to study the heat transfer coefficient and friction factor by using artificial roughness in the form of specially prepared inverted U-shaped turbulators on the absorber surface of an air heater duct. The roughened wall is uniformly heated while the remaining three walls are insulated. These boundary conditions correspond closely to those found in solar air heaters. The experiments encompassed the Reynolds number range from 3800 to 18000; ratio of turbulator height to duct hydraulic mean diameter is varied from, $e/D_h = 0.0186$ to 0.03986 ($D_h = 37.63$ mm and $e = 0.7$ to 1.5 mm) and turbulator pitch to height ratio is varied from, $p/e = 6.67$ to 57.14 ($p = 10$–40 mm). The angle of attack of flow on turbulators, $\alpha = 90°$ kept constant during the whole experimentation. The heat transfer and friction factor data obtained is compared with the data obtained from smooth duct under similar geometrical and flow conditions. As compared to the smooth duct, the turbulator roughened duct enhances the heat transfer and friction factor by 2.82 and 3.72 times, respectively. The correlations have been developed for area averaged Nusselt number and friction factor for turbulator roughened duct.

10/00343 Fabrication and processing of polymer solar cells: a review of printing and coating techniques

Krebs, F. C. *Solar Energy Materials and Solar Cells*, 2009, 93, (4), 394–412.

Polymer solar cells are reviewed in the context of the processing techniques leading to complete devices. A distinction is made between the film-forming techniques that are used currently such as spincoating, doctor blading and casting and the, from a processing point of view, more desirable film-forming techniques such as slot-die coating, gravure coating, knife-over-edge coating, off-set coating, spray coating and printing techniques such as ink jet printing, pad printing and screen printing. The former are used almost exclusively and are not suited for high-volume production whereas the latter are highly suited, but little explored in the context of polymer solar cells. A further distinction is made between printing and coating when a film is formed. The entire process leading to polymer solar cells is broken down into the individual steps and the available techniques and materials for each step are described with focus on the particular advantages and disadvantages associated with each case.

10/00344 Fabrication of buried contact silicon solar cells using porous silicon

Vitanov, P. *et al. Solar Energy Materials and Solar Cells*, 2009, 93, (3), 297–300.

This study reports the fabrication of buried contact solar cells using porous silicon as sacrificial layer to create well-defined channels (for buried contacts) in silicon. In this paper, the salient features of the technology have been presented. No detrimental effect was found in the performance of buried contact solar cell with partially filled contact area compared to the solar cells having conventional planar contacts. However, a marked difference in the short circuit current density was seen when channel was fully filled with metal by screen printing, without degradation in the open-circuit voltage. It is expected that improved processing in combination with optimized buried metallic contact parameters may yield higher efficiencies that may result in substantial decrease in solar cell cost.

10/00345 Hydrogen generation under sunlight by self ordered TiO_2 nanotube arrays

Liu, Z. *et al. International Journal of Hydrogen Energy*, 2009, 34, (8), 3250–3257.

Highly ordered TiO_2 nanotube arrays generate a considerable interest for hydrogen generation by an electrochemical photocell, since ordered architecture of nanotube arrays provides a unidirectional electric channel for electron's transport. Here, the authors report the hydrogen generation by highly ordered TiO_2 nanotube arrays under actual sunlight in KOH electrolyte. The two-electrode electrochemical cell included an adjustable anode compartment capable of tracing the trajectory of the sun and a set of alkaline batteries connected with a rheostat for application of external bias. The results showed that the photocurrent responses of nanotube arrays match well with the intensity of solar irradiance on a clear summer day. Addition of ethylene glycol into KOH electrolyte as a hole scavenger enhanced the rate of hydrogen generation. A maximum photocurrent density of 31 mA/cm^2 was observed at 13:30 h, by focusing the sunlight with an intensity of 113 mW/cm^2 on the surface of the TiO_2 nanotube arrays in 1 M KOH electrolyte with 10 vol% ethylene glycol under an applied bias of 0.5 V. The observed hydrogen generation rate was 4.4 mL/h cm^2 under the focalized solar irradiance with an intensity between 104 mW/cm^2 and 115 mW/cm^2 from 10:00 to 14:20 h.

10/00346 Impedance spectroscopy characterisation of highly efficient silicon solar cells under different light illumination intensities

Mora-Seró, I. *et al. Energy Environmental Science*, 2009, 2, (6), 678–686.

Highly efficient silicon solar cells have been characterized by impedance spectroscopy and current–potential characteristic in the dark and with different illumination intensities. For each illumination the impedance behaviour has been analysed at different applied bias potentials, in the forward and reverse region, comparing the results with the current–potential characteristic. Different cell parameters, as series and parallel resistances, capacitance, diode factor, minority carrier lifetime, acceptor impurities density and depletion layer charge density have been obtained as a function of bias voltage for different light illumination intensities. The effect of light-generated carriers and applied bias in the behaviour of the solar cell under illumination is discussed.

10/00347 Integrated blocking layers for hybrid organic solar cells

Memesa, M. *et al. Energy Environmental Science*, 2009, 2, (7), 783–790.

In hybrid organic solar cells a blocking layer between transparent electrode and nanocrystalline titania particles is essential to prevent short-circuiting and current loss through recombination at the electrode interface. Here the authors report the preparation of a thin, uniform and crack free hybrid blocking layer composed of conducting titania nanoparticles embedded in an insulating polymer derived ceramic. To do so sol–gel chemistry was combined with novel poly(dimethylsiloxane) containing amphiphilic block copolymer, poly(ethyleneglycol) methyl ether methacrylate–block–poly(dimethylsiloxane)–block–poly(ethyleneglycol) methyl ether methacrylate as the templating agent. Conductive probe scanning force microscopy proved that the existing percolating titania networks are separated by an insulating ceramic matrix. The structural uniformity of the percolating structures was investigated by microbeam grazing incidence small angle X-ray scattering making the integrated blocking layer suitable for hybrid organic solar device applications. Preliminary tests with the integrated blocking layer showed reasonable comparison to conventional TiO_2 blocking layer containing devices mentioned in the literature.

10/00348 Optimizing hybrid photovoltaics through annealing and ligand choice

Olson, J. D. *et al. Solar Energy Materials and Solar Cells*, 2009, 93, (4), 519–523.

Photovoltaic devices made from blended cadmium selenide nanocrystals with various capping ligands and poly-3-hexylthiophene were prepared. The effects of capping ligands and annealing conditions were investigated. It was found that capping ligands determine morphology/phase separation. These findings suggest that annealing at temperatures between 105 and 122 °C yield optimized devices. The authors also report CdSe/P3HT blended devices with an efficiency of 1.8% under illumination by AM1.5D.

10/00349 Performance analysis of a conventional PV/T mixed mode dryer under no load condition

Tiwari, G. N. *et al. International Journal of Energy Research*, 2009, 33, (10), 919–930.

A solar dryer integrated with photovoltaic powered DC fan has been designed and installed at Solar Energy Park, Indian Institute of Technology Delhi. The dryer has been coupled to a solar air heater having blackened surface of absorber for improved energy collection efficiency and a drying chamber with chimney. An analytical expression for characteristic equation for photovoltaic/thermal mixed mode dryer has been derived as a function of design and climatic parameters. The experiment was carried out for forced mode under no load conditions during April 2008 and validated with theoretical results for New Delhi climatic condition. This paper also shows the detailed analysis of thermal energy, exergy, and electrical energy gain by considering four weather conditions (a, b, c, and d type) for five different cities (New Delhi, Bangalore, Mumbai, Srinagar, and Jodhpur) of India.

10/00350 Photocatalytic overall water splitting with dual-bed system under visible light irradiation

Bae, S. W. *et al. International Journal of Hydrogen Energy*, 2009, 34, (8), 3243–3249.

Photocatalytic overall water splitting has been demonstrated with WO_3 for oxygen-producing photocatalysts (OPC), and Rh-doped $SrTiO_3$ for hydrogen-producing photocatalysts (HPC) in a simulated dual-bed system under visible light irradiation ($\lambda \geq 400$ nm). The Fe^{3+}/Fe^{2+} redox couple was chosen as the most effective electron mediator between OPC and HPC. The overall performance of the dual-bed system was limited by the low activity of HPC, and thus the activity of HPC should be increased to improve the overall performance. For the overall water splitting reaction in a dual-bed system, the conduction band of OPC must be more negative than the redox potential of the electron acceptors and the valence band of HPC must be more positive than the redox potential of the electron donors.

10/00351 Seasonal variation analysis of the outdoor performance of amorphous Si photovoltaic modules using the contour map

Nakada, Y. *et al. Solar Energy Materials and Solar Cells*, 2009, 93, (3), 334–337.

The effects of module temperature (T_{mod}) and spectral irradiance distribution on the outdoor performance of amorphous Si (a-Si) photovoltaic (PV) modules were investigated using contour maps. Compared to PV modules based on crystalline Si, such as single-crystalline Si (sc-Si) and multicrystalline Si, a-Si PV modules exhibit complex behaviour with seasonal variation. This study statistically analyses the outdoor performance of a-Si and sc-Si PV modules. The influence of environmental factors on outdoor performance of a-Si PV modules was analysed for two seasons, spring and autumn, in which the data periods had nearly the same average T_{mod} and integrated irradiation. The outdoor performance of the a-Si PV module depends on both temperature history and light-induced degradation.

Wind energy

10/00352 Considering wind speed correlation of WECS in reliability evaluation using the time-shifting technique

Xie, K. and Billinton, R. *Electric Power Systems Research*, 2009, 79, (4), 687–693.

Wind power is a very useful renewable energy source that is attracting consideration around the world due to its non-exhaustive nature and its environmental and social benefits. The correlation between multiple wind sites has a significant impact on the reliability of power systems containing wind energy conversion systems (WECS). Conventional methods cannot be directly applied to evaluate the reliability of WECS in the absence of comprehensive modelling techniques that recognize the correlation of the wind speeds at different wind farm locations. This paper proposes a model for power system reliability assessment that can consider the wind speed correlation and preserve the statistical characteristics of wind speeds, such as the mean and deviation of the wind speed time series (WSTS). A time-shifting technique is used to produce a new WSTS for a given correlation between two wind sites. The optimal shifted time at the two sites is determined using a linear interpolation technique. The probability distributions of the generated power and the system reliability indices with different degrees of correlation between the two sites are compared using two reliability test systems, i.e. the RBTS and the IEEE-RTS. The results show that the proposed method is useful in evaluating the reliability of WECS with correlation between two wind sites.

10/00353 Economical assessment of a wind–hydrogen energy system using WindHyGen® software

Aguado, M. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 2845–2854.

This paper considers the problem of analysing the economical feasibility of a wind–hydrogen energy storage and transformation system. Energy systems based on certain renewable sources as wind power, have the drawback of random input making them a non-reliable supplier of energy. Regulation of output energy requires the introduction of new equipment with the capacity to store it. Hydrogen was chosen as an energy storage system because of its versatility. The advantage of these energy storage systems is that the energy can be used (sold) when the demand for energy rises, and needs (prices) therefore are higher. There are two disadvantages: (a) the cost of the new equipment and (b) energy loss due to inefficiencies in the transformation processes. In this study, the authors developed a simulation model to aid in the economic assessment of this type of energy systems, which also integrates an optimization phase to simulate optimal management policies. Finally wind–hydrogen farm is analysed in order to determine its economical viability compared to current wind farms.

10/00354 Experimental and analytical studies of lightning overvoltages in wind turbine generator systems

Yamamoto, K. *et al. Electric Power Systems Research*, 2009, 79, (3), 436–442.

This paper presents the results of the experimental and analytical studies undertaken for the lightning protection of wind turbine generator systems by using a reduced-size wind turbine model. In the analytical studies, the finite difference time domain method is used. This study focuses on the overvoltages observed at the wavefronts of lightning surges. The lightning strokes on one of the blades and on the nacelle were considered, and the experiments and analyses were carried out by considering the cases of summer and winter lightning. The voltages and currents at various positions on the wind turbine model were considered.

10/00355 Wind energy conversion system regulation via LMI fuzzy pole cluster approach

Besheer, A. H. *et al. Electric Power Systems Research*, 2009, 79, (4), 531–538.

This paper addresses the design of a fuzzy state feedback controller that has not only the ability to stabilize the fuzzy model/system but also to control the transient behaviour and closed loop poles location for wind energy conversion system (WECS) that presents interesting control demands and exhibits intrinsic non-linear characteristics. The proposed fuzzy controller is employed to regulate indirectly the power flow in the grid connected WECS by regulating the DC current flows in the interconnected DC link. First, a Takagi–Sugeno fuzzy model is employed to represent the non-linear WECS. Then a model-based fuzzy controller design utilizing the concept of parallel-distributed compensation is developed. Satisfactory time response and closed loop damping over wide operating range are achieved by forcing the closed loop poles into a suitable sub-region of the complex frequency plane. Sufficient stability conditions are expressed in terms of linear matrix inequalities (LMIs) which can be solved very efficiently using convex optimization techniques. The design procedures are applied to a dynamic model of a typical wind energy conversion system to illustrate the feasibility and the effectiveness of the proposed control techniques via simulation example.

Others, including economics

10/00356 A new tailored scheme for the support of renewable energies in developing countries

Moner-Girona, M. *Energy Policy*, 2009, 37, (5), 2037–2041.

Historically the promotion of renewable energy technologies in isolated areas has involved international donors or governments subsidising the initial capital investment. This paper proposes an alternative support mechanism for remote villages based on the generation of renewable electricity. This communication presents an evaluation of the Renewable Energy Premium Tariff (RPT) scheme, a locally adapted variation of the feed-in tariff tailored for decentralized grids of developing countries. The RPT scheme stimulates the deployment of renewable energy technologies by paying for renewable electricity generated. A good-quality performance is secured since the support is given based on the electricity produced by renewables, not for the initial capital investment. The mechanism has been designed to provide a cost-effective scheme for the introduction of renewable energy technologies to remote villages, to provide sustainable and affordable electricity to local users, to make renewable energy projects attractive to policy-makers, and concurrently decrease financial risk to attract private sector investment.

10/00357 A new thinking for renewable energy model: remote sensing-based renewable energy model

Wang, S. *et al. International Journal of Energy Research*, 2009, 33, 778–786.

This paper mainly focuses on the two issues through remote sensing: assessment of the renewable energy potential and integration of the renewable energy model. Three methods for assessing the renewable energy potential with remote sensing (RS) are proposed. The methods can provide more precise evaluation of renewable energy potential, which is the first important step to develop a renewable energy model. The paper then first presents three integrations of the renewable energy model with RS and points out that with respect to the problems one of them is employed. The assessment methods based on RS and the integrations with RS are illustrated by a simple example with Europe solar energy data set. The results show that Germany is the optimal country to install photovoltaic with a capacity of 137 125 GW.

10/00358 A review on solar-hydrogen/fuel cell hybrid energy systems for stationary applications

Yilanci, A. *et al. Progress in Energy and Combustion Science*, 2009, 35, (3), 231–244.

There are several methods for producing hydrogen from solar energy. Currently, the most widely used solar hydrogen production method is to obtain hydrogen by electrolysing the water at low temperature. In this study, solar hydrogen production methods, and their current status, are assessed. Solar-hydrogen/fuel cell hybrid energy systems for stationary applications, up to the present day are also discussed, and preliminary energy and exergy efficiency analyses are performed for a photovoltaic-hydrogen/fuel cell hybrid energy system in Denizli, Turkey. Three different energy demand paths – from photovoltaic panels to the consumer – are considered. Minimum and maximum overall energy and exergy efficiencies of the system are calculated based on these paths. It is found that the overall energy efficiency values of the system vary between 0.88% and 9.7%, while minimum and maximum overall exergy efficiency values of the system are between 0.77% and 9.3% as a result of selecting various energy paths. More importantly, the hydrogen path appears to be the least efficient one due to the addition of the electrolyser, the fuel cells and the second inverter for hydrogen production and utilization.

10/00359 A snapshot of renewable energy research in Turkey

Celiktas, M. S. *et al. Renewable Energy*, 2009, 34, (6), 1479–1486.

The present study was conducted to find out the development trends of the scientific studies in the field of renewable energies in Turkey. All the publications in the ISI Web database were screened using 36 different keywords in title or topics based on the affiliation addresses including the word 'Turkey'. A total of 12,197 publications were processed article by article and as a result 1555 papers were found to focus on renewable energies between the years 1980 and 2008 with the contributions of 1605 authors. The results showed that 45.2% was experimental, 34.3% informational studies whereas 20.5% was available system analysis. Number of publications in biomass and conversion system (39.1%) and solar energy systems (20.0%) were dominating. Both number of publications and citations increased in the last decade and more than half of total contributions were published last four years. Results indicated that policy development studies (3.3%) were the weakest among the whole parameters investigated.

10/00360 Accelerating hydrogen implementation by mass production of a hydrogen bus chassis

Ally, J. and Pryor, T. *Renewable and Sustainable Energy Reviews*, 2009, 13, (3), 616–624.

Much of the hydrogen vehicle research to date has been conducted and demonstrated in wealthy nations, with very few exceptions. However, developing economies are largely dependent on public transportation, and struggle with air pollution and energy security concerns. The developing regions are in great need of alternative transportation solutions, and although many alternatives are being explored, hydrogen-fueled vehicles are emerging as one of the only technologies that can meet the demands for lower greenhouse gas emissions, lower emissions of air pollutants, and reduced dependence on imported energy. Many conventional buses in developing regions are built from an imported 'buggy-chassis', which is a functional bus chassis with an engine and other auxiliaries. 'Buggy-chassis' are designed with a very short wheel-base dimension to reduce freight costs as they are often shipped overseas. Domestic companies extend the 'buggy-chassis' to full bus length, build the body and cabin, and install other auxiliary systems. The existing infrastructure of the bus buggy-chassis market can be used to leverage hydrogen technology for mass production. This solution allows developing nations to import a state-of-the-art vehicle, with the possibility for local content in the final delivered product, while maintaining the flexibility for innovative technological developments and promoting hydrogen research within the developing economies. Indeed, a modular series-hybrid drivetrain can be made adaptable to a range of primary power sources such as an internal combustion engine or fuel cell engine. The modular approach provides an opportunity to reduce cost while still providing flexibility for innovation, and allows customers to tailor performance to suit their topographical and operational needs.

10/00361 Environmental mercantilism: how not to meet America's renewable energy targets

Krapels, E. N. *The Electricity Journal*, 2009, 22, (3), 13–16.

Ambitious renewables objectives can be met – without exposing ratepayers to cost overruns – but only if we harness the best of regulation and competition. An open and competitive process, leading to long-term power purchasing agreements, overseen by state and federal regulators, can get the job done.

10/00362 Nanoscale design to enable the revolution in renewable energy

Baxter, J. *et al. Energy Environmental Science*, 2009, 2, (6), 559–588.

The creation of a sustainable energy generation, storage, and distribution infrastructure represents a global grand challenge that requires massive transnational investments in the research and development of energy technologies that will provide the amount of energy needed on a sufficient scale and timeframe with minimal impact on the environment and have limited economic and societal disruption during implementation. This opinion paper focuses on an important set of solar, thermal, and electrochemical energy conversion, storage, and conservation technologies specifically related to recent and prospective advances in nanoscale science and technology that offer high potential in addressing the energy challenge. The authors approach this task from a two-fold perspective: analysing the fundamental physicochemical principles and engineering aspects of these energy technologies and identifying unique opportunities enabled by nanoscale design of materials, processes, and systems in order to improve performance and reduce costs. The principal goal is to establish a roadmap for research and development activities in nanoscale science and technology that would significantly advance and accelerate the implementation of renewable energy technologies. In all cases specific recommendations are made for research needs in the near-term (2–5 years), mid-term (5–10 years) and long-term (>10 years), as well as projecting a timeline for maturation of each technological solution. The authors also identify a number of priority themes in basic energy science that cut across the entire spectrum of energy conversion, storage, and conservation technologies. It is anticipated that the conclusions and recommendations herein will be of use not only to the technical community, but also to policy makers and the broader public, occasionally with an admitted emphasis on the US perspective.

10/00363 Structure of turbulent flow in EMEC's tidal energy test site

Osalusi, E. *et al. International Communications in Heat and Mass Transfer*, 2009, 36, (5), 422–431.

Measurements of bulk turbulent parameters (kinetic energy, dissipation rates, Reynolds stress, etc.) were performed in the bottom boundary layer of the European Marine Energy Centre (EMEC) tidal test site using Acoustic Doppler Current Profilers (ADCPs). Flood and ebb currents exceed $1.4\,\mathrm{ms}^{-1}$ near the seabed (at 2.63 mab) and generate $>7\,\mathrm{Pa}$ stresses. The production of turbulent kinetic energy (TKE) P, was found to be negative below $2\times10^{-9}\,\mathrm{Wm}^{-3}$ and, of up to $5\times10^{-4}\,\mathrm{Wm}^{-3}$ was estimated during flood flows and decreasing to $10^{-5}\,\mathrm{Wm}^{-3}$ during slack water. The TKE dissipation rate ϵ was estimated using the structure function method with greatest value of up to $5\times10^{-1}\,\mathrm{Wm}^{-3}$ near the seabed around maximum flood, falling to $4\times10^{-3}\,\mathrm{Wm}^{-3}$ around slack water. The comparison between P and ϵ was performed by calculating individual ratios of P corresponding to ϵ using a bootstrap resampling technique. The study shows that the ratio ϵ/P averaged over whole flood and ebb were found to be ~0.3553 and ~0.3266, respectively, indicating that production exceeds dissipation. The uncertainties in Reynolds stress estimates due to instrument noise was found to be $4\times10^{-4}\,\mathrm{Pa}$.

14 FUEL SCIENCE AND TECHNOLOGY

Fundamental science, analysis, instrumentation

10/00364 An experimental study of bouncing Leidenfrost drops: comparison between Newtonian and viscoelastic liquids

Bertola, V. *International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1786–1793.

The effect of polymer additives on the dynamic Leidenfrost phenomenon (rebound of liquid drops impacting on very hot walls, where a thin vapour cushion separates the liquid from the surface) is studied experimentally by high-speed imaging. Drops of a dilute solution (200 ppm) of polyethylene oxide (PEO), with equilibrium diameters of 2.66 and 3.32 mm, were compared with drops of pure water (diameters of 2.76 and 3.49 mm) during the impact on an aluminium surface at a temperature of 400 °C and impact Weber numbers between 7 and 160. The additive causes a slight reduction of the maximum spreading diameter and of the retraction velocity of the drop after impact and, within a certain range of Weber numbers, enhances significantly the maximum height of the drop centre of mass during rebound. These results, obtained for a non-wetting case, are different from those previously obtained for impacts on dry surfaces, where polymer additives hardly change the maximum spreading diameter but reduce the retraction velocity of nearly one order of magnitude and completely suppress drop rebound.

10/00365 A computerized tool to evaluate the cognitive compatibility of the emergency operational procedures task flow

Carvalho, P. V. R. *et al. Progress in Nuclear Energy*, 2009, 51, (3), 409–419.

Nuclear power production is a safety-critical process where ultimate decisions lie with the operators. During postulated incidents and accidents, operators rely on emergency operational procedures (EOPs), which are the most used decision support tool. This study presents a method to develop a computerized tool, based on the ACT-R cognitive architecture, to evaluate the logical task flow in the EOPs, verifying if the timing assumptions for operator's actions contained in the procedure scripts can be accomplished by the human operators. The tool is used to model the nuclear power plant (NPP) operator crew tasks during a loss of coolant accident (LOCA) simulation. To validate the procedural scripts, the tool calculates the time intervals that operators need to accomplish actions and compare these time intervals with the plant dynamic behaviour during the evolution of the accident. The tool proved to be an adequate way to validate the logical task flow of the EOP analysed, showing that operators have enough time to execute their actions and an adequate waiting (free) time between some of their actions. The developed tool provides a low cost alternative solution for NPPs owners and regulatory bodies to validate the logical task flow and quality issues of the hundreds of NPPs procedures.

10/00366 A one-dimensional model of vertical gas plume migration through a heterogeneous porous medium

Silin, D. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (3), 300–310.

This work is motivated by the growing interest in injecting carbon dioxide into deep geological formations as a means of avoiding its atmospheric emissions and consequent global warming. Ideally, the injected greenhouse gas stays in the injection zone for a geologic time, eventually dissolves in the formation brine and remains trapped by mineralization. However, one of the potential problems associated with the geologic method of sequestration is that naturally present or inadvertently created conduits in the cap rock may result in a gas leakage from primary storage. Even in supercritical state, the carbon dioxide viscosity and density are lower than those of the formation brine. Buoyancy tends to drive the leaked CO_2plume upward. Theoretical and experimental studies of buoyancy-driven supercritical CO_2 flow, including estimation of time scales associated with plume evolution and migration, are critical for developing technology, monitoring policy, and regulations for safe carbon dioxide geologic sequestration. In this study, the authors obtain simple estimates of vertical plume propagation velocity taking into account the density and viscosity contrast between CO_2 and brine. They describe buoyancy-driven countercurrent flow of two immiscible phases by a Buckley–Leverett type model. The model predicts that a plume of supercritical carbon dioxide in a homogeneous water-saturated porous medium does not migrate upward like a bubble in bulk water. Rather, it spreads upward until it reaches a seal or until it becomes immobile. A simple formula requiring no complex numerical calculations describes the velocity of plume propagation. This solution is a simplification of a more comprehensive theory of countercurrent plume migration. In a layered reservoir, the simplified solution predicts a slower plume front propagation relative to a homogeneous formation with the same harmonic mean permeability. In contrast, the model yields much higher plume propagation estimates in a high-permeability conduit like a vertical fracture.

10/00367 A three-dimensional inverse geometry problem in estimating the space and time-dependent shape of an irregular internal cavity

Huang, C.-H. and Chen, C.-A. *International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 2079–2091.

A three-dimensional inverse geometry problem (or shape identification problem) to estimate the unknown space and time-dependent irregular shape of internal cavity by utilizing the gradient-based steepest descent method (SDM) and a general purpose commercial code CFD-ACE+ is considered in the present study. The validity of the present inverse algorithm is examined based on the simulated measured temperature distributions on the outer surface by an imaginary infrared scanner. The advantage of calling CFD-ACE+ as a subroutine in this shape identification problem lies in its characteristics of automatic mesh generation since this function of CFD-ACE+ enables the easily handling of the moving boundary problem. Two numerical test cases are performed to test the validity and accuracy of the present shape identification algorithm by using different types of cavity shapes, initial guesses and measurement errors. Results show that excellent estimations on the unknown geometry of the internal cavity can be obtained.

10/00368 Applications of computational intelligence techniques for solving the revived optimal power flow problem

AlRashidi, M. R. and El-Hawary, M. E. *Electric Power Systems Research*, 2009, 79, (4), 694–702.

Computational intelligence tools are attracting added attention in different research areas and research in power systems is not different. This paper provides an overview of major computational issues with regard to the optimal power flow (OPF). Then, it offers a brief summary of major computational intelligence tools. A detailed coverage of most OPF related research work that make use of modern computational intelligence techniques is presented next.

10/00369 Combined cyclic voltammetry and in situ electrochemical atomic force microscopy on lead electrode in sulfuric acid solution with or without lignosulfonate

Hirai, N. *et al. Journal of Power Sources*, 2009, 191, (1), 97–102.

The effect of lignosulfonate (LS) on electrochemical reaction of lead electrode (as a model of negative electrode) has been investigated in 1 M, 3 M, or 7.1 M H_2SO_4 aqueous solution with 0, 10, 100 or 1000 mg l^{-1} of LS using cyclic voltammetry (CV) combined with *in situ* electrochemical atomic force microscopy (EC-AFM), as well as rotating ring disk electrode. The anodic peaks of the CVs, which correspond to overall reaction of $Pb + SO_4^{2-} \rightarrow PbSO_4 + 2e^-$, shifted positive when LS was added or the concentration of H_2SO_4 was lower. The anodic capacities of the CVs increased with addition of LS when the concentration of H_2SO_4 was lower. When LS was added, the anodic capacities of the CVs usually increased especially in less concentrated H_2SO_4 solution at higher sweep rate, while the anodic capacity slightly decreased in 7.1 M H_2SO_4 solution with addition of LS at sweep rate of 10 mV min^{-1}; that is, in most concentrated H_2SO_4 solution at lower sweep rate in this paper. Two cathodic peaks of the CVs were observed when LS was added, and the peak at lower potential shifted more negative with increase of LS. Lead sulfate crystals dissolved at more negative potential with increase of LS. LS up-took Pb^{2+} ions in H_2SO_4 aqueous solution during discharging.

10/00370 Computation accuracy and efficiency of a power series analytic method for two- and three-space-dependent transient problems

Aboanber, A. E. and Hamada, Y. M. *Progress in Nuclear Energy*, 2009, 51, (3), 451–464.

The establishment of solutions to large-scale three-dimensional (3-D) reactor benchmark problems is needed to serve as standards for the verification of design codes and for the detailed error analysis of calculational methods. A number of partially and fully inserted control rods, represented by absorber added to certain subassemblies, cause a strong nonseparable power distribution. In addition, the existence of a very large thermal flux peak in the reflector makes this a very difficult and challenging problem to solve. PWS code has been developed to include a numerical solution for the time-dependent neutron diffusion equations for the nuclear reactor analysis. The new technique employs a new parameter (α) which can reduce the rapid increase in magnitude of the power series coefficients. These coefficients, in turn, are determined by back substitutions in the non-linear canonical diffusion equations and treating terms of the same degree to obtain a modified recurrence relation which is valid for any type of the stiff non-linear kinetic diffusion equations. The validity of the algorithm was tested with three kinds of well-known two-group benchmark problems. The first one is the two-dimensional TWIGL seed-blanket reactor kinetics problem. The second is the two- and three-dimensional LAR BWR benchmark problem simulating a rod drop accident of a BWR core. The third is the three-dimensional LMW LRA transient problem which simulates an operational transient involving rod movements. The obtained results with the proposed PWS code are compared with those provided by other reference codes, indicating an overall agreement and excellent performance.

10/00371 Development of a model for calculating the longwave optical properties and surface temperature of a curved Venetian blind

Chaiyapinunt, S. and Worasinchai, S. *Solar Energy*, 2009, 83, (6), 817–831.

This article is about the development of a mathematical model for calculating the longwave optical properties of a curved Venetian blind. The calculated optical properties are used to determine the performance of the glass window installed with a Venetian blind in terms of thermal comfort. The blind, whose optical properties are considered non-specular, is modelled as an effective layer. The effect of slat curvature is included in the developed model. A six surface enclosure formed by two consecutive slats is used to analyse for the longwave optical properties of the effective layer. The longwave optical properties, transmittance, reflectance, absorptance and emittance are developed by using the radiosity method. The steady state energy balance method along with the developed longwave optical properties are used to determine the surface temperature of the effective layer. The empirical expression for the total heat flux from the indoor glass window surface with an adjacent Venetian blind is adopted in the developed model. The surface temperature of the blind, which is the key parameter for calculating the thermal performance of glass windows with venetian blinds with respect to thermal comfort, is chosen as the parameter used for the model validation. The predicted surface temperature of the Venetian blind is compared with the surface temperature of the Venetian blind obtained from the measurement. The agreement between the predicted temperature and the measured temperature is good.

10/00372 Development of the three-dimensional numerical generation of response factors method of conductive temperatures in passive cooling earth-contact components

Zoras, S. and Kosmopoulos, P. *Solar Energy*, 2009, 83, (6), 862–872.

This paper reports on the development and application of a method for the numerical prediction of temperatures within passive cooling components. In previous studies the basic idea was presented in an alternate form for the prediction of earth-contact heat transfer. The new method incorporates elements of the response factor method into a finite volume technique based numerical model. Initially, a 'pre-processing' procedure is required to generate a certain number of hours for use as a time series by the response factor technique in the second stage of the method. It is here shown that even a reduced number of temperature response factors, e.g. 50 h, is sufficient to obtain accurate predictions of the component's hourly temperature profile up to 1 year ahead. This study develops the equations addressing temperature profiles in structural components. The 'state of the art' of the presented method corresponds in the way that the conductive temperature response factors are calculated being numerically in the three-dimensional space. The method solves the three-dimensional earth-contact temperature profiles, which interact with indoors and outdoors temperature profiles. Once the numerical temperature response factors time series of an earth-contact component's grid node have been generated then its future thermal performance due to any surrounding temperature variation can be predicted fast and accurately. The structural earth-contact passive cooling components' response factors are generated by a three-dimensional numerical model, with no need of past experimental data and stored to be used at any time in future. The method is given the name numerical generation of response factors. The way that the temperature response factors are determined in the three-dimensional space targets in the improvement of the prediction of earth-contact temperature profiles.

10/00373 e-Science in high energy density science research

Nishihara, K. *et al. Fusion Engineering and Design*, 2009, 83, (2–3), 525–529.

This study presents three achievements related to e-Science in high energy density science research. The authors developed a test module of new database system for nation-wide users of the high power lasers at Osaka University with web technology, a flexible control system and an XML-database, which provide efficient, accurate and flexible R&D processing. They also constructed a EUV-GRID portal system for integrated computer simulations of laser produced plasma–extreme ultraviolet (LPP–EUV) light source development, which provides a flexible framework for automatic sequencing of workflow for the integrated simulations. A dynamical domain decomposition method in molecular dynamic (MD) simulations is required to obtain a good adaptive load balancing for heterogeneous computing environments such as grid, a new algorithm of this was also developed. The authors successfully performed large scale MD-message passing interface (MPI) simulations on cluster computers connected through Super-SINET using the National Research Grid Initiative (NAREGI GRID) grid middleware and the new algorithm.

10/00374 Effect of sample shape on counter-current spontaneous imbibition production *vs* time curves

Mason, G. *et al. Journal of Petroleum Science and Engineering*, 2009, 66, (3–4), 83–97.

Counter-current spontaneous imbibition experiments on porous media are usually carried out using cylindrical core samples. Sometimes the cores are sealed on some of the faces, and experiments then give production curves of significantly different duration and slightly different shape. Results can be correlated for rock properties (porosity and permeability) and fluid properties (viscosity and interfacial tension). A single overall scale factor is usually used to correlate for different core sizes and shapes. Although the real imbibition process is actually quite complicated, by making the approximations that there is (a) frontal displacement and (b) constant saturation behind the front, a simple analytical solution is possible. The analysis gives the production vs time function and a new core shape scale factor. These assumptions also allow the scale factors of Ma et al. to be used to predict the shape of the production vs time curves. In order to challenge the predictions of the production vs time curves and the Ma, Ruth and new scale factors, counter-current spontaneous imbibition experiments were carried out with matched oil-saturated cores of different shape using brine to spontaneously displace the mineral oil. Amongst others, cylindrical cores with an axial hole were used with either the inner or outer cylindrical face open. These have radial geometry with imbibition into a contracting or expanding volume. Analysis of the experimental results with the new theory confirmed that the Ma and Ruth scale factors are good to excellent for most situations but that the new one is marginally better for extreme shape variations. The theory also predicts that all of the results should be linked by a universal properties factor (*G*). The variability of the *G* factor can be explained by some of the cores not having enough exposed surface and not enough rock depth. These factors seem to be of greater importance than the differences between the scale factors. For reproducible results it appears that a core should have an imbibition face area of at least 40 cm^2 and a thickness (open face to no-flow boundary) of at least 1 cm.

10/00375 Experimental and numerical investigation of non-predictive phase-control strategies for a point-absorbing wave energy converter

Lopes, M. F. P. *et al. Ocean Engineering*, 2009, 36, (5), 386–402.

Phase control may substantially increase the power absorption in point-absorber wave energy converters. This study deals with validation of dynamic models and latching control algorithms for an oscillating water column (OWC) inside a fixed vertical tube of small circular cross-section by small-scale testing. The paper describes experimental and numerical results for the system's dynamics, using simple and practical latching control techniques that do not require the prediction of waves or wave forces, and which will be relevant to any type of point-absorbing devices. In the experimental set-up, the upper end of the tube was equipped with an outlet duct and a shut-off valve, which could be controlled to give a latching of the inner free surface movement. The pressure drop through the open valve is used as a simplified measure of the energy extraction. The control was realized by using the real-time measurement signals for the inner and outer surface displacement. A mathematical model of the system was established and applied in numerical simulation. In the case the OWC's diameter is much smaller than the wavelength and the wave amplitude much smaller than the draft, the free surface movement inside the tube can be described as an oscillating weightless piston. For this hydrodynamic problem an analytical solution is known. In addition, the mathematical model includes the effects of viscous flow losses, the air compressibility inside the chamber and the pressure drop across the valve. Experimental results were used to calibrate some of the model parameters, and the total model was formulated as a coupled system of six non-linear, first-order differential equations. Time-domain integration was used to simulate the system in order to test the control strategies and compare with experimental results.

10/00376 Fast camera imaging of dust in the DIII-D tokamak

Yu, J. H. *et al. Journal of Nuclear Materials*, 2009, 390–391, 216–219.

Naturally occurring and injected dust particles are observed in the DIII-D tokamak in the outer midplane scrape-off-layer (SOL) using a visible fast-framing camera, and the size of dust particles is estimated using the observed particle lifetime and theoretical ablation rate of a carbon sphere. Using this method, the lower limit of detected dust radius is ~3 μm and particles with inferred radius as large as ~1 mm are observed. Dust particle 2D velocities range from approximately 10 to 300 m/s with velocities inversely correlated with dust size. Pre-characterized 2–4 μm diameter diamond dust particles are introduced at the lower divertor in an ELMing H-mode discharge using the divertor materials evaluation system (DiMES), and these particles are found to be at the lower size limit of detection using the camera with resolution of ~0.2 cm^2 per pixel and exposure time of 330 μs.

10/00377 Flow towards a guarded sampling probe: modelling of a 2D flow cell

Sherwood, J. D. *Journal of Petroleum Science and Engineering*, 2009, 66, (3–4), 133–142.

Analytic and numerical methods are used to predict fluid flow in a thin rectangular sheet of porous material when fluid is extracted through a port at the midpoint of one of the edges of the sheet. The aim is to model (in two dimensions) flow towards a sampling probe used to extract reservoir fluids from the rock surrounding a newly drilled well. Such samples are usually contaminated with drilling fluid filtrate that saturates the rock adjacent to the wellbore, but a guarded probe can eliminate this contamination. Complex variable techniques are used to determine the flow of incompressible fluids when the interface between the two fluids is sharp, and filtrate and original pore fluid have identical viscosities. Results are compared against the predictions of a numerical reservoir simulator, and agreement is reasonable once numerical dispersion has been accounted for. Numerical results are also obtained for the case when the viscosities of the two fluids differ. The results give confidence in the use of 3-dimensional numerical computations to predict flow towards a guarded probe in a real wellbore, and thereby to optimize the design of such probes.

10/00378 Fuzzy-based methodology for performance assessment of emergency planning and its application

Chen, G. and Zhang, X. *Journal of Loss Prevention in the Process Industries*, 2009, 22, (2), 125–132.

Emergency planning is the guidance in emergency responses and its performance can influence the whole rescue process. Hence aiming at improving the emergency planning performance and further promoting the rescue efficiency, there is an urgent requirement to appraise the performance of emergency planning. A mature emergency system is the premise to ensure emergency planning to be performed perfectly. First, the maturity of emergency system is evaluated qualitatively by comparing the challenge caused by potential risk and emergency capability formed by emergency system. If the emergency capability can encounter the potential risk, the emergency system is viewed as mature. Second, functional attributes are analysed and the performance assessment index system of emergency planning is set up by characterizing the attributes in detail. Third, according to the hierarchical characteristics of the index system, the performance assessment method for emergency planning is put forward through the combination of Analytic Hierarchy Process (AHP) and fuzzy theories. In the method, defuzzification is introduced so as to achieve the integrated performance of emergency planning and performance taxis of all assessment indices. The taxis from priority to inferiority of performance indices can be used as references to improve the emergency planning. Finally, the application of the method in a petrochemical materials storage depot indicates that the disadvantages existing in the emergency system and emergency planning can be found out through the assessment results and the advices given to the depot improve the emergency system maturity and the emergency planning performance.

10/00379 Investigation of karst collapse based on 3-D seismic technique and DDA method at Xieqiao coal mine, China

Zuo, J. P. *et al. International Journal of Coal Geology*, 2009, 78, (4), 276–287.

Karst collapse is a serious geological problem in most of the coal mines in the north of China, but recently it has been found in the south as well. The present study is aimed at investigating subsidence mechanism and deformation field of a karst collapse column at Xieqiao, in the south of China. A method of three-dimensional (3-D) seismic technique has been successful in exploring the spatial morphology of the karst collapse at Xieqiao, and the discontinuous deformation analysis (DDA) method is used to calculate the deformation field and analyse the subsidence mechanism. The results indicated that DDA could approximately simulate and back analyse the subsidence process and strata deformation fields. The subsidence processes of the collapse column depend on the sizes of the karst caves. With the continuous expansion of the karst caves, a semi-elliptic stress field, local separation strata and fracture zone will be formed around the karst cave. Moreover, they will gradually expand upwards along the vertical direction. The paper also indicates that the subsidence failure stage may trigger a sudden collapse of the karst column because of the sudden energy release. Also, it will make a great impact on the vicinity working face so as to cause a rock burst. The effects of the friction angle of rock strata on the subsidence mechanism were reported firstly based on DDA.

10/00380 Investigation of the effect of chemistry models on the numerical predictions of the supersonic combustion of hydrogen

Kumaran, K. and Babu, V. *Combustion and Flame*, 2009, 156, (4), 826–841.

In this numerical study, the influence of chemistry models on the predictions of supersonic combustion in a model combustor is investigated. To this end, 3D, compressible, turbulent, reacting flow calculations with a detailed chemistry model (with 37 reactions and nine species) and the Spalart–Allmaras turbulence model have been carried out. These results are compared with earlier results obtained using single step chemistry. Hydrogen is used as the fuel and three fuel injection schemes, namely, strut, staged (i.e. strut and wall) and wall injection, are considered to evaluate the impact of the chemistry models on the flow field predictions. Predictions of the mass fractions of major species, minor species, dimensionless stagnation temperature, dimensionless static pressure rise and thrust percentage along the combustor length are presented and discussed. Overall performance metrics such as mixing efficiency and combustion efficiency are used to draw inferences on the nature (whether mixing- or kinetic-controlled) and the completeness of the combustion process. The predicted values of the dimensionless wall static pressure are compared with experimental data reported in the literature. The calculations show that multi step chemistry predicts higher and more widespread heat release than what is predicted by single step chemistry. In addition, it is also shown that multi step chemistry predicts intricate details of the combustion process such as the ignition distance and induction distance.

10/00381 Numerical analysis of thermal striping induced high cycle thermal fatigue in a mixing tee

Lee, J. I. *et al. Nuclear Engineering and Design*, 2009, 239, (5), 833–839.

Thermal striping, characterized by turbulent mixing of two flow streams of different temperatures that result in temperature fluctuations of coolant near the pipe wall, is one of the main causes of thermal fatigue failure. Coolant temperature oscillations due to thermal striping are on the order of several Hz. Thermal striping high-cycle thermal fatigue that occurs at tee junctions is one of the topics that should be addressed for the life management of light water reactor (LWR) piping systems. This study focuses on numerical analyses of the temperature fluctuations and structural response of coolant piping at a mixing tee. The coolant temperature fluctuations are obtained from Large Eddy Simulations that are validated by experimental data. For the thermal stress fatigue analysis, a model is developed to identify the relative importance of various parameters affecting fatigue-cracking failure. This study shows that the temperature difference between the hot and cold fluids of a tee junction and the enhanced heat transfer coefficient due to turbulent mixing are the dominant factors of thermal fatigue failure of a tee junction.

10/00382 On the consistency of mechanistic multidimensional modelling of gas/liquid two-phase flows

Podowski, M. Z. *Nuclear Engineering and Design*, 2009, 239, (5), 933–940.

The purpose of this paper is to present an overview of selected aspects of the mathematical modelling of multiphase flows, including the formulation of governing equations, gas/liquid interfacial forces and bubble/bubble interactions. Links between the combined physical, mathematical and computational models are discussed, including the recent progress in, and the limitations of, computational multiphase fluid dynamics (CMFD). Major differences and similarities are analysed between the interpenetrating-fluids multifield modelling concept and the model of dispersed two-phase flows. Conditions are formulated under which the multifield modelling framework is applicable to gas/liquid dispersed bubbly flows. Also, the interactions between the continuous and dispersed fields are discussed, including a new mechanistic modelling concept for the turbulence-induced interfacial forces between the continuous liquid and dispersed bubbles. Finally, a multigroup approach to the modelling of bubble coalescence and breakup is presented.

10/00383 Retrieval of thermal properties in a transient conduction–radiation problem with variable thermal conductivity

Das, R. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2749–2758.

This article reports an inverse analysis of a transient conduction–radiation problem with variable thermal conductivity. Simultaneous retrieval of parameters is accomplished by minimizing the objective function represented by the square of the difference between the measured and the assumed temperature fields. The measured temperature field is calculated from the direct method involving the lattice Boltzmann method (LBM) and the finite volume method (FVM). In the direct method, the FVM is used to obtain the radiative information and the LBM is used to solve the energy equation. With perturbations imposed on the measured temperature data, minimization of the objective function is achieved with the help of the genetic algorithm. The accuracies of the retrieved parameters have been studied for the effects of the genetic parameters such as the crossover and the mutation rates, the population size, the number of generations and the effect of noise on the measured temperature data. A good estimation of parameters has been obtained.

10/00384 Robust hydrogen detection system with a thermoelectric hydrogen sensor for hydrogen station application

Nishibori, N. *International Journal of Hydrogen Energy*, 2009, 34, (6), 2834–2841.

A prototype hydrogen detection system using the micro-thermoelectric hydrogen sensor (micro-THS) was developed for the safety of hydrogen infrastructure systems, such as hydrogen stations. The authors have designed a detection part with a pressure proof enclosure adoptable for the international standard of Exd II CT3, and carried out an explosion strength test, explosion and fire hazard tests, and an impact test. The hydrogen sensing performance of the detection part of this prototype system showed a good linear relationship between the sensing signal and hydrogen concentrations in air, for a wide range of hydrogen concentrations from 10 ppm to 40,000 ppm (4 vol.%). This prototype detection system was installed in the outdoor field of the hydrogen station and the response for H_2 gas in air of 100 ppm, 1000 ppm, and 10000 ppm was tested monthly for 1 year.

10/00385 Study of the sensitivity of a thermal flow sensor

Kim, T. H. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 2140–2144.

The sensitivity of a thermal flow sensor is investigated in this study. A simple numerical model for analysing heat transfer phenomena in the thermal flow sensor is presented. In order to validate the proposed model, experimental investigations are performed. Based on the results from the validated model, a correlation that predicts the sensitivity of the thermal flow sensor is presented. From the correlation, the manner in which the heat loss, the positions of the temperature sensors, the input power, and the heater length affect the sensitivity of the thermal flow sensor is investigated.

10/00386 Theoretical studies on polynitro-1,3-bishomopentaprismanes as potential high energy density compounds

Qiu, L. *et al. Journal of Hazardous Materials*, 2009, 166, (2–3), 931–938.

Based on the fully optimized molecular geometric structures at the DFT-B3LYP/6–31G* level, the densities (ρ), detonation velocities (D) and pressures (P) for a series of polynitro-1,3-bishomopentaprismanes (PNBPPs), as well as their thermal stabilities, were investigated to look for high energy density compounds (HEDCs). The studied PNBPPs have high values of heats of formation (HOFs) and the magnitude is correlative with the number (n) and the space distance of nitro groups. D and P for PNBPPs were estimated by using modified Kamlet–Jacobs equations based on the calculated HOFs and ρ. It is found that ρ, D and P all increase with n and satisfy the group additivity rule. The calculations on the bond dissociation energies of C–NO_2 and C–C bonds indicate that both bonds are possible to be the trigger bond in the pyrolysis process, and this interesting phenomenon is related with the molecular structure, especially the strain energy of the skeleton. In conjunction with the energetic performances and thermal stabilities, PNBPPs with $n = 8$–12 are recommended as the preferred candidates of HEDCs. These results would provide basic information for the further studies of PNBPPs.

10/00387 Three-dimensional simulation of turbulent forced convection in a duct with backward-facing step

Lan, H. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1690–1700.

Results from three-dimensional (3-D) simulations of turbulent forced convection adjacent to backward-facing step in a rectangular duct using a k-ϵ-ζ-f turbulence model are reported. This turbulence model is numerically robust near the wall, and it has been shown to predict turbulent heat transfer in separated and wall-bounded flows better than commonly used two-equation turbulence models. FLUENT-CFD code is used as the platform for these simulations and User Defined Functions (UDF) are developed for incorporating this turbulence model into the code. The UDF implementation is validated by simulating several 2-D separated flow/heat transfer benchmark problems. The resulting excellent agreements between the simulated results and benchmark data for these 2-D problems justify the use of this resource for simulating 3-D convection problems. Three-dimensional backward-facing step geometry with an expansion ratio of 1.48 and with a step height of 4.8 mm is used in this study. Three aspect ratios of 3, 8 and infinity (2-D simulation) are considered for studying its effect on the flow and heat transfer, and similarly the effect of the Reynolds number was examined by varying its magnitude in the range of 20,000–50,000. Simulated results are presented for the general 3-D flow features, the reattachment lines, temperature and Nusselt number distributions that develop in this geometry.

10/00388 Topology optimization for thermal conductors considering design-dependent effects, including heat conduction and convection

Iga, I. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2721–2732.

In structural designs considering thermal loading, in addition to heat conduction within the structure, the heat convection upon the structure's surface can significantly influence optimal design configurations. This paper focuses on the influence of design-dependent effects upon heat convection and internal heat generation for optimal designs developed using a topology optimization scheme. The method for extracting the structural boundaries for heat convection loads is constructed using a Hat function, and heat convection shape dependencies are taken into account in the heat transfer coefficient using a surrogate model. Several numerical examples are presented to confirm the usefulness of the proposed method.

Fuel cell technology

10/00389 A new parameter extraction method for accurate modelling of PEM fuel cells

Outeiro, M. T. *et al. International Journal of Energy Research*, 2009, 33, (11), 978–988.

In this paper, a new parameter extraction method for accurate modelling of proton exchange membrane (PEM) fuel cell systems is presented. The main difficulty in obtaining an accurate PEM fuel cell dynamical model is the lack of manufacturer information about the exact values of the parameters needed for the model. In order to obtain a realistic dynamic model of the PEM system, the electrochemical considerations of the system are incorporated into the model. Although many models have been reported in the literature, the parameter extraction issue has been neglected. However, model parameters must be precisely identified in order to obtain accurate simulation results. The main contribution of the present work is the application of the simulated annealing (SA) optimization algorithm as a method for identification of PEM fuel cell model parameter identification. The major advantage of SA is its ability to avoid becoming trapped in local minimum, as well as its flexibility and robustness. The parameter extraction and performance validation are carried out by comparing experimental and simulated results. The good agreement observed confirms the usefulness of the proposed extraction approach together with adopted PEM fuel cell model as an efficient tool to help design of power fuel cell power systems.

10/00390 A numerical investigation of modelling an SOFC electrode as two finite layers

Hussain, M. M. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 3134–3144.

Modelling an electrode in solid oxide fuel cells (SOFCs) as two finite layers was investigated numerically. A simulation was conducted using the developed mathematical model, wherein an SOFC electrode is considered as a porous composite structure of electron- and ion-conducting particles. Moreover, an electrochemical reaction is considered to occur throughout the electrode. In other words, an electrode is treated as a reaction zone layer having triple phase boundaries (TPBs) scattered throughout the electrode, consistent with the micro modelling approach of treating electrodes. The model takes into account the transport of multi-component mixture in an electrode together with electrochemical reaction, the transport of electrons and ions in the respective electron-conducting and ion-conducting particles of the electrode. It is found that both the dimensionless electronic and ionic current densities remain constant with respective values of one and zero for most part of the anode before started to vary towards the end of the anode. Further, from the distributions of dimensionless electronic and ionic current densities in the anode, it can be deduced that the part of the anode (electrode) where the value of dimensionless electronic current density is one, can be considered as an electron-conducting (ion insulator) layer, referred to as the anode (electrode) backing layer; the part of the anode (electrode), where there is a variation in the electronic and ionic current densities and electrochemical reaction rate is most effective, can be considered as a mixed-conducting layer, referred to as the reaction zone layer. Finally, a parametric study is conducted to investigate the effect of key operating and design conditions on the thickness of the reaction zone layer in an SOFC anode.

10/00391 A prototype of a fuel cell PEM emulator based on a buck converter

Marsala, G. *et al. Applied Energy*, 2009, 86, (10), 2192–2203.

The fuel cell system (FCS), including all its auxiliaries and related control systems, is emulated by a buck converter realized experimentally and controlled in the DSPACE environment. The realization of the buck converter allows the behaviour of any fuel cells to be easily emulated since only the modification of the control law of the switch is necessary. The proposed emulator can be applied easily to other fuel cell systems if the polarization curve has the same current rate and maximum power. In this way it is possible to utilize the converter and perform optimization tests without wasting hydrogen or purchasing cells, as well as avoiding any cell damage. With regard to current other types of emulators, the one presented here has the following characteristics: (1) all the auxiliaries of the system have been considered, each includes its own control system, as in a real FCS, (2) the converter is a classical buck converter with a free-wheeling diode and is designed to have a high bandwidth and to be practically always in conduction mode (discontinuous mode appears only at very low currents), (3) the voltage control is made by a space-state controller, able to fix properly the closed loop poles of the system, thus guaranteeing the desired bandwidth of the control system and (4) it can be used in laboratory as a stand-alone low-cost system for design and experimental purposes.

10/00392 Ammonia-fed solid oxide fuel cells for power generation – a review

Ni, M. *et al. International Journal of Energy Research*, 2009, 33, (11), 943–959.

Ammonia has been identified as a promising sustainable fuel and hydrogen source for solid oxide fuel cells (SOFC). This paper provides a literature review on ammonia-fed SOFCs. Both experimental studies and mathematical modelling investigations on NH_3-fed SOFC are included and discussed. It is found that NH_3 is a technically feasible fuel for direct use in SOFCs and the performance of NH_3-fed SOFC is comparable with that of the H_2 fed SOFC. Experimental study in literature also demonstrates that both oxygen ion-conducting electrolyte (SOFC-O) and proton-conducting electrolyte (SOFC-H) can be used in NH_3-fed SOFC, as the amount of NO_x generated in a SOFC-O is negligible. Fabricating thin film electrolyte and developing more reactive electrode materials are important to improve the performance of NH_3-fed SOFCs. Mathematical models are useful design tools for understanding the coupled transport and reaction phenomena and for optimizing the SOFC performance. The authors have developed, validated and demonstrated reliable thermodynamic and pioneering 1D electrochemical models.

10/00393 Assessment of factors responsible for polymer electrolyte membrane fuel cell electrode performance by statistical analysis

Velayutham, G. *et al. Journal of Power Sources*, 2009, 191, (1), 10–15.

The performance of the fuel cell electrode depends on many factors: types of materials and their properties, composition, process parameters and fuel cell operation conditions. In the present paper, cathode electrode performance in a PEM fuel cell as a function of Teflon concentration in the substrate materials and in micro-layer carbon, pore former in the micro-layer, amount of carbon used in the diffusion layer and platinum/nafion loading in the catalyst layer are studied. These six factors each at two levels are considered. A full factorial design would have required 2^6, i.e. 64 experiments to be carried out. With the use of Taguchi method, L_{12} designs, the number of experiments can be reduced to 12. The electrode current density values are taken as responses for the analysis. Statistical sensitivity analysis (ANOVA analysis) is used to compute the effects and the contributions of the various factors to the fuel cell electrode. Some graphic representations are employed in order to display the results of the statistical analysis made for different current values. The behaviour of cathode PEM fuel cell electrode was studied using humidified hydrogen and compressed air. The present paper examines the six main factors and their levels responsible for altering the performance particularly when the fuel is operated under ambient pressure.

10/00394 Cobalt oxide supported on alumina catalysts prepared by various methods for use in catalytic afterburner of PEM fuel cell

Zacharaki, I. *et al. Catalysis Today*, 2009, 143, (1–2), 38–44.

This study investigated the influence of the preparation method on the physicochemical and activity features of cobalt oxide catalysts used for the combustion of anode tail gas produced in a proton-exchange membrane (PEM) fuel cell. The catalysts prepared contain 21% (w/w) Co and have been calcined at 850 °C. Three different impregnation methodologies have been followed: incipient wetness impregnation (IWI) using a cobalt nitrate aqueous solution, incipient wetness impregnation using a mixed cobalt nitrate–nitrilotriacetic acid (IWI-nta) aqueous solution and equilibrium deposition filtration (EDF) using a cobalt nitrate aqueous solution. The EDF methodology imposed interfacial deposition and resulted to the formation of an almost bi-dimensional surface precipitate. Upon calcination, this surface precipitate provided a very well-dispersed CoO_x amorphous species strongly interacted with the support surface and thus hardly reducible as well as relatively small Co_3O_4 supported nanocrystals (14.3 nm). The first phase is the predominant one. Therefore, EDF resulted to a catalyst with the highest cobalt surface and specific surface area. The conventional IWI imposed bulk (solution) precipitation and thus induced relatively large supported crystallites which upon calcination provided relatively large supported Co_3O_4 nanocrystals (19.8 nm) and $CoAl_2O_4$ as well. The formation of the relatively large nanocrystals and the insertion of cobalt inside the γ-alumina lattice to form $CoAl_2O_4$ may be responsible for the lowest cobalt surface obtained in this catalyst. The presence of the nitrilotriacetic acid in the impregnating solution induced the exchange of the water ligands of the Co(II) aqua complex present in the cobalt nitrate solution with organic ligands and thus the bulk precipitation of an organometallic complex. The more bulky organic ligands decreased the cobalt-support interactions. Thus, the insertion of cobalt inside the γ-alumina lattice and the formation of $CoAl_2O_4$ are inhibited upon calcination of the IWI-nta sample. This may be responsible for the relatively higher cobalt surface obtained with respect to that achieved in the IWI sample though the size of the Co_3O_4 nanocrystals is larger in the IWI-nta sample (25.8 nm). At relatively high reaction temperatures all catalysts exhibited almost the same activity for oxidation reactions. In contrast, at low reaction temperatures the EDF catalyst proved to be more active for the CH_4 production as well as for the oxidation of H_2 and CO. This behaviour may be attributed to the favourable physicochemical characteristics of this catalyst.

10/00395 Electrical contact resistance between stainless steel bipolar plate and carbon felt in PEFC: a comprehensive study

André, J. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 3125–3133.

Bipolar plate represents a key component of proton exchange membrane fuel cell (PEFC) with several essential functions, among them the electric connection of elementary cells. Usually made of graphite, this component is studied worldwide in order to develop a commercially viable alternative: different ways have been being investigated, and to date, despite corrosion issues, stainless steel (SS) appears as a good candidate material, but its Electrical Contact Resistance (ECR) can reach unacceptable values when exposed to PEFC environment. This paper offers a comprehensive study of the parameters acting on ECR when using uncoated SS in PEFC: roughness, which influences the surface contact area with carbon baking, bulk composition of the alloy, which influences only partly the nature of passive films, and the composition and structure of passive films, strongly modified by surface treatments and ageing conditions.

10/00396 Electrochemical evidence of direct electrode reduction by a thermophilic Gram-positive bacterium, *Thermincola ferriacetica*

Marshall, C. W. *et al.* May, H. D. *Energy Environmental Science*, 2009, 2, (6), 699–705.

Microbial fuel cells (MFCs) are bioelectrochemical devices capable of converting chemical energy to electrical energy using bacteria as the catalysts. Mechanisms of microbial electron transfer to solid electrode surfaces are not well defined in most electrochemically-active microorganisms, particularly for Gram-positive bacteria. This study investigated the electrochemical characteristics of the Gram-positive, thermophilic bacterium *Thermincola ferriacetica* strain Z-0001. This organism was capable of transferring electrons from acetate to the anode of an MFC to generate an electric current. *T. ferriacetica* exhibited rapid recovery of current following medium exchanges, recovering to near-maximum current output in less than three hours. The recovery of electrons from acetate was 97% in air-cathode MFCs inoculated with *T. ferriacetica*. Further insights into the anode reduction by these biofilms were gained through cyclic voltammetry (CV). A continuous steady-state current was reached above -0.1 V vs Ag/AgCl reference electrode in CV scans of an established *T. ferriacetica* biofilm. A catalytic wave with a midpoint potential consistently near -0.28 V indicated a continuous electron-transporting interface between the attached microbial biofilm and the electrode surface. Additionally, no significant peaks were observed when scanning cell-free spent medium from active MFCs. These data suggest that *T. ferriacetica* directly transfers electrons to an electrode through a mechanism that is tightly associated with the biofilm that forms on the electrode. This is the first mechanistic insight into how Gram-positive extracellular electron transfer might occur without the addition of soluble electron shuttling mediators. These mechanistic evaluations will be essential for the improvement and application of such biocatalysts in microbial fuel cells and other bioelectrochemical systems.

10/00397 Fluid-dynamic characterisation of MCFC gas distributors

Marra, D. *et al. Chemical Engineering and Processing: Process Intensification*, 2009, 48, (3), 797–807.

Previous studies at the plant scale have shown that thermal management is a crucial point in molten carbonate fuel cell operation optimization. At the local scale, the principal mechanisms controlling the temperature map on the cell plane have been analysed and it has been shown that the fluid dynamics of the anodic and cathodic gases on the cell could have a fundamental role in thermal optimization. So, the authors have analysed the gas flow in planner cells, using a computational fluid dynamics (CFD) technique and identifying the characteristic fluid-dynamic parameters. The studied structure consists of a typical current collector/gas distributor formed by a plurality of arches with suitable height to provide sufficient reactant flow area, proper stiffness to accept compressive load and adequate resiliently to distribute the load and maintain electrical contact. The results of this analysis are presented and discussed in this paper, while the modelling approach is presented as a useful tool for improving the current collector/gas distributor design, identifying new technological solutions and optimizing MCFC performance.

10/00398 Fuel cell electrodes using carbon nanostructures

Lebert, M. *et al. Catalysis Today*, 2009, 143, (1–2), 64–68.

The use of carbon nanotubes (CNTs) for low and intermediate temperature fuel cells has been investigated with thin film CNT/Pt-electrodes of ($1 < d < 10\,\mu m$). For membrane electrode assembly (MEA) the electrodes were combined either with Nafion® 117 or polycarbonate (PC) membranes wetted with H_3PO_4. The fuel cell characteristics of the CNT-based MEAs were determined at atmospheric pressure, different catalyst concentrations (Pt) and temperatures ($RT < T < 150\,°C$). The performance is competitive to well-established phosphoric acid fuel cells (PAFCs) or polymer electrolyte membrane fuel cells (PEMFC), e.g. PBI/H_3PO_4. Liquid state processing of CNTs allows flexible electrode design and opens new ways for integrated and significantly mass-/volume-reduced fuel cell electrodes with high saving potential for catalyst and carbon material. Microsized high performance power supplies and battery chargers for consumer electronics are the most promising applications.

10/00399 Hydrogen purification using compact pressure swing adsorption system for fuel cell

Majlan, E. H. *et al. International Journal of Hydrogen Energy*, 2009, 34, (6), 2771–2777.

Adsorption of CO and CO_2 in mixtures of H_2/CO/CO_2 was achieved using compact pressure swing adsorption (CPSA) system to produce purified hydrogen for use in fuel cell. A CPSA system was designed by combining four adsorption beds that simultaneously operate at different processes in the pressure swing adsorption (PSA) process cycle. The overall diameter of the cylindrical shell of the CPSA is 35 cm and its height is 40 cm. Several suitable adsorbent materials for CO and CO_2 adsorption in a hydrogen stream were identified and their adsorption properties were tested. Activated carbon from Sigma-Aldrich was the adsorbent chosen. It has a surface area of $695.07\,m^2/g$. CO adsorption capacity (STP) of 0.55 mmol/g and CO_2 at 2.05 mmol/g were obtained. The CPSA system has a rapid process cycle that can supply hydrogen continuously without disruption by the regeneration process of the adsorbent. The process cycle in each column of the CPSA consists of pressurization, adsorption, blowdown and purging processes. CPSA is capable of reducing the CO concentration in a H_2/CO/CO_2 mixture from 4000 ppm to 1.4 ppm and the CO_2 concentration from 5% to 7.0 ppm CO_2 in 60 cycles and 3600 s. Based on the mixture used in the experimental work, the H_2 purity obtained was 99.999%, product throughput of 0.04 kg H_2/kg adsorbent with purge/feed ratio was 0.001 and vent loss/feed ratio was 0.02. It is therefore concluded that the CPSA system met the required specifications of hydrogen purity for fuel cell applications.

10/00400 Mass transport phenomena in direct methanol fuel cells

Zhao, T. S. *et al. Progress in Energy and Combustion Science*, 2009, 35, (3), 275–292.

Clean and highly efficient energy production has long been sought to solve energy and environmental problems. Fuel cells, which convert the chemical energies stored in fuel directly into electrical energy, are expected to be a key enabling technology for this century. This article is concerned with one of the most advanced fuel cells – direct methanol fuel cells (DMFCs). A comprehensive review of the state-of-the-art studies of mass transport of different species is presented, including the reactants (methanol, oxygen and water) and the products (water and carbon dioxide) in DMFCs. Rather than elaborating on the details of the previous numerical modelling and simulation, the article emphasizes: (i) the critical mass-transport issues that need to be addressed so that the performance and operating stability of DMFCs can be upgraded, (ii) the basic mechanisms that control the mass-transport behaviours of reactants and products in this type of fuel cell, and (iii) the previous experimental and numerical findings regarding the correlation between the mass transport of each species and cell performance.

10/00401 Measurement of flow maldistribution in parallel channels and its application to ex-situ and in-situ experiments in PEMFC water management studies

Kandlikar, S. G. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1741–1752.

Uniform flow distribution is critical to obtaining high performance in many heat and mass transfer devices. It also plays an important role in the effective operation of a proton exchange membrane fuel cell (PEMFC). In this work, a novel technique based on the entrance region pressure drop measurements is presented for monitoring fluid flow maldistribution in individual channels. The method is validated using liquid water flow in a test section with four tubes in parallel, and then applied to assess the air flow maldistribution in PEMFCs using (a) an *ex situ* experimental setup simulating the two-phase flow in parallel channels, and (b) an *in situ* experimental setup with an operating fuel cell. While an almost uniform air distribution is obtained for the parallel channels with an impermeable backing (plastic sheet), severe maldistribution is observed for the same channels with porous GDL backing. The maldistribution caused by the water blockage in an *ex situ* test setup is further investigated and the results are verified by the high-speed images of the two-phase flow in channels. The technique has also been applied in an *in situ* experimental setup to obtain the flow maldistribution under electrochemical reaction conditions in the presence of two-phase flow in the cathode side gas channels.

10/00402 Microporous layer for water morphology control in PEMFC

Nam, J. H. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (11–12), 2779–2791.

This study used an environmental scanning electron microscope to observe vapour condensation and liquid water morphology and breakthrough in porous layers of polymer electrolyte membrane fuel cell. These suggest the presence of large droplets and high liquid saturation at interface of the catalyst layer (CL) and gas diffusion layer (GDL), due to a jump in pore size. The authors developed a model for morphology of the liquid phase across multiple porous layers by use of both continuum and breakthrough (percolation) treatments. Using the results of this model, the authors show the liquid morphologies deteriorating the efficiency of electrochemical reactions in CL and increasing the water saturation in GDL. The authors also show that inserting a microporous layer between CL and GDL reduces both the droplet size and liquid saturation and improves the cell performance.

10/00403 PEMFC electrode preparation by electrospray: optimization of catalyst load and ionomer content

Chaparro, A. M. *et al. Catalysis Today*, 2009, 143, (3–4), 237–241.

Electrodes for proton exchange membrane fuel cell (PEMFC) have been prepared by means of electrospray deposition, using different ionomer contents and catalyst loads. The electrodes have been mounted in single PEMFC, and tested as cathode. The electroactive platinum area of electrosprayed electrodes has been measured by the hydrogen underpotential deposition method. Polarization curves have been measured to determine the optimal concentration for the platinum catalyst (Pt/C, 20 wt%) and the ionomer (Nafion®). Best performance is observed with 15% ionomer content in the electrosprayed cathode due to minimal cell internal resistance. This optimal concentration is lower than that found for electrodes prepared by other standard methods, like airbrushing or impregnation, which is attributed to the improved ionomer distribution within the electrospray deposited catalyst layer. On the other hand, the optimum value for catalyst load is similar to that encountered for electrodes prepared by the other methods, which reflects that electrospray has little or no effect neither on the catalyst nor on the electronic resistance of the catalyst layer.

10/00404 The effect of current density and temperature on the degradation of nickel cermet electrodes by carbon monoxide in solid oxide fuel cells

Offer, G. J. and Brandon, N. P. *Chemical Engineering Science*, 2009, 64, (10), 2291–2300.

The oxidation of dry carbon monoxide (CO) in intermediate temperature solid oxide fuel cells (IT-SOFCs) has been studied using a three electrode assembly. Ni/CGO:CGO:LSCF/CGO three electrode pellet cells at 500, 550 and 600 °C were exposed to dry carbon monoxide for fixed periods of time, at open circuit and under load at 50 and $100\,mA\,cm^{-2}$, in an aggressive test designed to accelerate electrode degradation. It is shown that if the anode is kept under load during exposure to dry CO, degradation in anode performance can be minimized, and that under most conditions the anode showed significant irreversible degradation in performance after subsequent load cycling on dry H_2. Only at 500 °C and at $100\,mA\,cm^{-2}$ was the degradation in performance after operation on dry CO and subsequent load cycling on dry H_2 within the background degradation rates measured. Where anode performance was compromised, this appeared to be caused by a reduction in the exchange current density for hydrogen oxidation, and the relatively large degradation after load cycling on dry H_2 was primarily caused by an increase in the series resistance of the anode. It is suggested that this increase in series resistance is associated with the removal of carbon deposited in the non-electrochemically active region of the electrode during operation on dry CO, and that operation under load inhibits carbon deposition in the active region.

10/00405 Two-dimensional modelling of electrochemical and transport phenomena in the porous structures of a PEMFC

Sahraoui, M. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 3091–3103.

A two-dimensional CFD model of PEM fuel cell is developed by taking into account the electrochemical, mass and heat transfer phenomena occurring in all of its regions simultaneously. The catalyst layers and membrane are each considered as distinct regions with finite thickness and calculated properties such as permeability, local protonic conductivity, and local dissolved water diffusion. This finite thickness model enables to model accurately the protonic current in these regions with higher accuracy than using an infinitesimal interface. In addition, this model takes into account the effect of osmotic drag in the membrane and catalyst layers. General boundary conditions are implemented in a way taking into consideration any given species concentration at the fuel cell inlet, such as water vapour which is a very important parameter in determining the efficiency of fuel cells. Other operating parameters such as temperature, pressure and porosity of the porous structure are also investigated to characterize their effect on the fuel cell efficiency.

10/00406 Water management studies in PEM fuel cells, part I: Fuel cell design and in situ water distributions

Owejan, J. P. *et al. International Journal of Hydrogen Energy*, 2009, 34, (8), 3436–3444.

A proton exchange membrane fuel cell (PEMFC) must maintain a balance between the hydration level required for efficient proton transfer and excess liquid water that can impede the flow of gases to the electrodes where the reactions take place. Therefore, it is critically important to understand the two-phase flow of liquid water combined with either the hydrogen (anode) or air (cathode) streams. This paper describes the design of an *in situ* test apparatus that enables investigation of two-phase channel flow within PEMFCs, including the flow of water from the porous gas diffusion layer (GDL) into the channel gas flows; the flow of water within the bipolar plate channels themselves; and the dynamics of flow through multiple channels connected to common manifolds which maintain a uniform pressure differential across all possible flow paths. These two-phase flow effects have been studied at relatively low operating temperatures under steady-state conditions and during transient air purging sequences.

10/00407 Water management studies in PEM fuel cells, part II: Ex situ investigation of flow maldistribution, pressure drop and two-phase flow pattern in gas channels

Lu, Z. *et al. International Journal of Hydrogen Energy*, 2009, 34, (8), 3445–3456.

Two-phase flow of water and reactant gases in the gas distribution channels of proton exchange membrane fuel cells (PEMFCs) plays a critical role in proper water management. In this work, the two-phase flow in PEMFC cathode parallel channels is studied over a wide range of superficial air velocity (air stoichiometry) and superficial water velocity in a specially designed *ex situ* experimental setup, which enables the measurement of instantaneous flow rates in individual gas channels and simultaneous visualization of the water flow structure. It is found that the two-phase flow at low superficial air velocities (air stoichiometry < 5) is dominated by slugs or semi-slugs, leading to severe flow maldistribution and large fluctuations in the pressure drop. Slug residence time, measured from the video observation and the instantaneous flow rate data, is found to be a new parameter to describe the slug flow. At higher air velocities, a water film is formed on the channel walls if they are hydrophilic. The pressure drop for the film flow is characterized by smaller but frequent fluctuations, which are found to result from the water buildup at the channel-exit manifold interface. As the superficial air velocity increases further, mist flow is obtained where little water buildup is observed. The water buildup in the gas channels at the two-phase flow is well described by the two-phase friction multiplier, defined as the ratio of the two-phase pressure drop to the single gas phase pressure drop. It is found that the two-phase friction multiplier increases with increasing water flow rate. A flow pattern map is developed using superficial water and air velocities with clearly defined transition regions.

15 ENVIRONMENT

Pollution, health protection, applications

10/00408 3D geomechanical modelling for CO_2 geologic storage in the Dogger carbonates of the Paris Basin

Vidal-Gilbert, S. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (3), 288–299.

CO_2 injection into a depleted hydrocarbon field or aquifer may give rise to a variety of coupled physical and chemical processes. During CO_2 injection, the increase in pore pressure can induce reservoir expansion. As a result the *in situ* stress field may change in and around the reservoir. The geomechanical behaviour induced by oil production followed by CO_2 injections into an oil field reservoir in the Paris Basin has been numerically modelled. This paper deals with an evaluation of the induced deformations and *in situ* stress changes, and their potential effects on faults, using a 3D geomechanical model. The geomechanical analysis of the reservoir–caprock system was carried out as a feasibility study using pressure information in a 'one way' coupling, where pressures issued from reservoir simulations were integrated as input for a geomechanical model. The results show that under specific assumptions the mechanical effects of CO_2 injection do not affect the mechanical stability of the reservoir–caprock system. The ground vertical movement at the surface ranges from -2 mm during oil production to $+2.5$ mm during CO_2 injection. Furthermore, the changes in *in situ* stresses predicted under specific assumptions by geomechanical modelling are not significant enough to jeopardize the mechanical stability of the reservoir and caprock. The stress changes issued from the 3D geomechanical modelling are also combined with a Mohr–Coulomb analysis to determine the fault slip tendency. By integrating the stress changes issued from the geomechanical modelling into the fault stability analysis, the critical pore pressure for fault reactivation is higher than calculated for the fault stability analysis considering constant horizontal stresses.

10/00409 Application of bioemulsifiers in soil oil bioremediation processes. Future prospects

Calvo, C. *et al. Science of the Total Environment*, 2009, 407, (12), 3634–3640.

Biodegradation is one of the primary mechanisms for elimination of petroleum and other hydrocarbon pollutants from the environment. It is considered an environmentally acceptable way of eliminating oils and fuel because the majority of hydrocarbons in crude oils and refined products are biodegradable. Petroleum hydrocarbon compounds bind to soil components and are difficult to remove and degrade. Bioemulsifiers can emulsify hydrocarbons enhancing their water solubility and increasing the displacement of oily substances from soil particles. For these reasons, inclusion of bioemulsifiers in a bioremediation treatment of a hydrocarbon polluted environment could be really advantageous. There is a useful diversity of bioemulsifiers due to the wide variety of producer microorganisms. Also their chemical compositions and functional properties can be strongly influenced by environmental conditions. The effectiveness of the bioemulsifiers as biostimulating agent in oil bioremediation processes has been demonstrated by several authors in different experimental assays. For example, they have shown to be really efficient in combination with other products frequently used in oil bioremediation such as they are inorganic fertilizer (NPK) and oleophilic fertilizer (i.e. S200C). On the other hand, the bioemulsifiers have shown to be more efficient in the treatment of soil with high percentage of clay. Finally, it has been proved their efficacy in other biotechnological processes such as *in situ* treatment and biopiles. This paper reviews literature concerning the application of bioemulsifiers in the bioremediation of soil polluted with hydrocarbons, and summarizes aspects of the current knowledge about their industrial application in bioremediation processes.

10/00410 Can a carbon permit system reduce Spanish unemployment?

Fæhn, T. *et al. Energy Economics*, 2009, 31, (4), 595–604.

This paper analyses the impact of carbon policy on unemployment in Spain and whether recycling the public revenues earned from permit auctions can alleviate this problem. While Spain's deviation from the European Union's intermediate emission goals is more serious than most other member countries' unemployment in Spain is also well above average for the European Union. A computable general equilibrium model is used that includes unemployment in the markets for unskilled and skilled labour. It is found that introducing carbon permits does not aggravate Spanish unemployment. In fact, if supplied with revenue recycling schemes, unemployment rates may actually fall. Contrary to other European studies, it is found that the best option is to reduce payroll taxes on relatively skilled types of labour. This reform is successful in both increasing labour demand and dampening the supply response to rising wages. However, while all of the recycling schemes generate dividends in terms of aggregate welfare, none entirely offsets the abatement costs.

10/00411 Chemical and ecotoxicological characterization of solid residues produced during the co-pyrolysis of plastics and pine biomass

Bernardo, M. S. *et al. Journal of Hazardous Materials*, 2009, 166, (1), 309–317.

A mixture of 70% (w/w) pine biomass and 30% (w/w) plastics (mixture of polypropylene, polyethylene, and polystyrene) was subjected to pyrolysis at 400 °C, for 15 min, with an initial pressure of 40 MPa. Part of the solid residue produced was subjected to extraction with dichloromethane (DCM). The extracted residue (residue A) and raw residue (residue B) were analysed by weight loss combustion and submitted to the leaching test ISO/TS 21268–2 using two different leachants: DCM (0.2%, v/v) and calcium chloride (0.001 mol/L). The concentrations of the heavy metals Cd, Cr, Ni, Zn, Pb and Cu were determined in the eluates and in the two residues. The eluates were further characterized by determining their pH and the concentrations of benzene, toluene, ethylbenzene and xylenes (BTEX). The presence of other organic contaminants in the eluates was qualitatively evaluated by gas chromatography, coupled with mass spectrometry. An ecotoxicological characterization was also performed by using the bio-indicator *Vibrio fischeri*. The chemical and ecotoxicological results were analysed according to the French proposal of Criteria on the Evaluation Methods of Waste Ecotoxicity (CEMWE). Residue A was not considered to be ecotoxic by the ecotoxicological criterion (EC_{50} (30 min) $\geq 10\%$), but it was considered to be ecotoxic by the chemical criterion ($Ni \geq 0.5$ mg/L). Residue B was considered to be ecotoxic by the ecotoxicological criterion: EC_{50} (30 min) $\leq 10\%$. Besides that, residue B was considered to be hazardous according the European legislation (BTEX concentrations higher than 100 ppb). The results indicate that volatile organic contaminants can be present in sufficient amounts in these residues and their eluates to induce ecotoxicity levels. The extraction of the pyrolysis residue with DCM was an efficient method for removing lighter organic contaminants.

10/00412 Depletion of forest resources in Sudan: intervention options for optimal control

Hassan, R. *et al. Energy Policy*, 2009, 37, (4), 1195–1203.

Agricultural expansion and over-cutting of trees for fuelwood are important causes of deforestation in arid and semi-arid countries such as Sudan. The consequence is increased desertification and high erosion and loss of soil nutrients leading to declining agricultural productivity. However, the social costs of the deforestation externality are not taken into account in present forest management and land use planning in Sudan leading to under-pricing and over-exploitation of the country's forest resources. This study evaluated the suitability of approaches commonly used by most forest resource management agencies for prediction of the state and control of harvesting of forest resources against alternative empirical simulation models using relevant information about economic behaviour of trading agents in the fuelwood market. Results showed the clear superiority of models integrating market behaviour over current approaches in the ability to better simulate real trends of wood consumption and hence depletion rates. The study also adopted an optimal control model to derive socially optimal forest harvesting regimes. The results showed that current rates of forest resource rent recovery and reforestation efforts are very far from optimal. Results also suggest that, in addition to optimal pricing and higher reforestation efforts, promotion and availability of fuel substitutes and investment in wood energy conversion efficiencies have a strong potential for curbing the problem of deforestation in Sudan.

10/00413 Determinants of variation in household CO_2 emissions between and within countries

Kerkhof, A. C. *et al. Energy Policy*, 2009, 37, (4), 1509–1517.

Variation in household CO_2 emissions between and within countries may have important consequences for the equity dimension of climate policies. In this study the aim is to identify some determinants of national household CO_2 emissions and their distribution across income groups. For that purpose, the CO_2 emissions of households in the Netherlands, UK, Sweden and Norway are quantified around the year 2000 by combining a hybrid approach of process analysis and input–output analysis with data on household expenditures. The results show that average households in the Netherlands and the UK give rise to higher amounts of CO_2 emissions than households in Sweden and Norway. Moreover, CO_2 emission intensities of household consumption decrease with increasing income in the Netherlands and the UK, whereas they increase in Sweden and Norway. A comparison of the national results at the product level points out that country characteristics, like energy supply, population density and the availability of district heating, influence variation in household CO_2 emissions between and within countries.

10/00414 Developing a green building assessment tool for developing countries – case of Jordan

Ali, H. H. and Al Nsairat, S. F. *Building and Environment*, 2009, 44, (5), 1053–1064.

The purpose of this research is to contribute to a better understanding of the concept of green building assessment tool and its role for achieving sustainable development through developing an effective green building rating system for residential units in Jordan in terms of the dimensions through which sustainable development tools are being produced and according to the local context. Developing such system is becoming necessary in the Developing World because of the considerable environmental, social and economical problems. Jordan as one of these countries is in need for this system, especially with poor resources and inefficient use. Therefore, this research studied international green building assessment tools such as such as LEED, CASBEE, BREEAM, GBTool, and others. Then defined new assessment items respecting the local conditions of Jordan and discussed them with (60) various stakeholders; 50% of them were experts of sustainable development. After selecting the assessment items they were weighted using the AHP method. The outcome of the research was a suggested green building assessment tool (SABA Green Building Rating System) – computer based program – that suits the Jordanian context in terms of environmental, social and economical perspectives.

10/00415 Dispersion by wind of CO_2 leaking from underground storage: comparison of analytical solution with simulation

Schwarz, K. T. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (4), 422–430.

The concentration of CO_2 in air near the ground needs to be predicted to assess environmental and health risks from leaking underground storage. There is an exact solution to the advection–diffusion equation describing trace gases carried by wind when the wind profile is modelled with a power-law dependence on height. The analytical solution is compared with a numerical simulation of the coupled air–ground system with a source of CO_2 underground at the water table. The two methods produce similar results far from the boundaries, but the boundary conditions have a strong effect; the simulation imposes boundary conditions at the edge of a finite domain while the analytic solution imposes them at infinity. The reverse seepage from air to ground is shown in the simulation to be very small, and the large difference between time scales suggests that air and ground can be modelled separately, with gas emissions from the ground model used as inputs to the air model.

10/00416 Dispersion of a buoyant plume in a turbulent pressure-driven channel flow

Fabregat, A. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (7–8), 1827–1842.

Direct numerical simulations of the turbulent dispersion of a buoyant line of hot fluid released at the inlet of a plane channel flow are reported ($Ret = 180$, $Gr = 10^7$ and $Pr = 0.7$). Results of turbulent dispersion of a neutrally buoyant scalar and mixed convection flow are also included. The buoyancy force induces a vertical movement that, although small in mean, exhibits a significant fluctuation in the vertical velocity component and deflects the plume with the consequent loss of symmetry found in the neutrally buoyant results. The modification of the budgets for the time averaged momentum and heat transport equations reflects the rearranging of the different contributions induced by the buoyancy force.

10/00417 Economics of climate change under uncertainty: benefits of flexibility

Anda, J. *et al. Energy Policy*, 2009, 37, (4), 1345–1355.

The selection of climate policy has to be made in an extremely uncertain environment: both benefits and costs of a particular climate policy are unknown and in the best case could be described by the probability distribution of various outcomes. Dominated in literature, the expected value approach to the cost–benefit analysis of climate policy under uncertainties relies on the aggregated estimation of various outcomes of climate policy weighted and averaged by probabilities. The variance, skewness, and kurtosis are important characteristics of uncertainties but can be easily lost in the process of aggregation. The real option analysis (ROA) explicitly accounts for both the expected value of underling assets and the variance of the expected value (as well as skewness and kurtosis that are important to describe a fat tail phenomenon). In the paper, an application of the real option analysis is proposed in order to formulate rules for the selection of a climate policy (emission target) and estimate the economic value of the future flexibility created by interim climate policy, which may be corrected in the future in response to new knowledge that hopefully reduces uncertainties. The initially selected interim policy has an option value and methodology for its valuation presented in the paper.

10/00418 Environmental efficiency in residential buildings – a simplified communication approach

Malmqvist, T. and Glaumann, M. *Building and Environment*, 2009, 44, (5), 937–947.

For all actors involved with planning, developing and managing buildings, the environmental impact relating to energy use and the quality of the indoor environment are both aspects of major concern. It is crucial that a reduction in the environmental impact of a building is not achieved through compromising the indoor environment. This paper presents a method to assess user satisfaction related to the indoor environment and the environmental impact related to the energy use of the building, i.e. the environmental efficiency of the building. This environmental efficiency comprises two indices that are calculated separately but displayed in the same diagram to facilitate communication of complex information. This approach forms part of the Swedish life cycle based environmental assessment tool for buildings, EcoEffect. The present paper presents and exemplifies the environmental efficiency of buildings using data from 26 Swedish multi-family residential buildings and proposes a number of reference values. The concept can be used as an overarching objective for environmental management of a property firm's building stock or for evaluating targets set in the planning process for a new building. It can also be used for environmental rating of buildings, which would probably increase the communication value further. The aggregated indices are rough but proportionately straightforward to calculate and easily communicated. In addition, they address the environmental impacts of buildings in a much more comprehensive way than the current practice.

10/00419 Environmental policies in a differentiated oligopoly revisited

Fujiwara, K. *Resource and Energy Economics*, 2009, 31, (3), 239–247.

Constructing a model of polluting oligopoly with product differentiation, it is considered how product differentiation, together with the presence and absence of free entry, affects optimal pollution tax/subsidy policies. The sign of the short- and long-run optimal pollution taxes are highly sensitive to the parameter measuring product differentiation as well as the presence of free entry. How they are affected by a change in product differentiation, which is not addressed in the existing literature, is also made clear.

10/00420 Ethnicity, housing and personal factors as determinants of VOC exposures

D'Souza, J. C. *et al. Atmospheric Environment*, 2009, 43, (18), 2884–2892.

Previous studies investigating effects of personal, demographic, housing and other factors on exposures to volatile organic compounds (VOC) have focused on mean or median exposures, and generally not the high exposures that are of great interest. This paper identifies determinants of personal VOC exposures on a quantile-specific basis using a nationally representative sample. The NHANES 1999–2000 VOC dataset was merged with personal, demographic, housing, smoking and occupation variables. Bivariate analyses tested for differences in geometric means and quantiles across levels of potential exposure determinants. Multivariate sample-weighted ordinary least-squares and quantile regression (QR) models were then used to adjust for covariates. A number of exposure determinants were identified, most of which varied by exposure quantile. The most striking finding was the much higher exposures experienced by Hispanics and Blacks for aromatic VOCs (BTEX: benzene, toluene, ethylbenzene and xylenes), methyl *tert*-butyl ether (MTBE), and 1,4-dichlorobenzene (DCB). Exposure to gasoline, paints or glues, and having a machine-related occupation also were associated with extremely high BTEX and MTBE exposures. Additional determinants included the presence of attached garages and open windows, which affected exposures of BTEX (especially at lower quantiles) and MTBE (especially at higher quantiles). Smoking also increased BTEX exposures. DCB was associated with air freshener use, and PERC with dry-cleaned clothing. After adjusting for demographic, personal and housing factors, age and gender were not significant predictors of exposure. The use of QR in conjunction with OLS yields a more complete picture of exposure determinants, and identifies subpopulations and heterogeneous exposure groups in which some individuals experience very elevated exposures and which are not well represented by changes in the mean. The high exposures of Hispanics and Blacks are perplexing and disturbing, and they warrant further investigation.

10/00421 Evaluating California local land use plan's environmental impact reports

Tang, Z. *et al. Environmental Impact Assessment Review*, 2009, 29, (2), 96–106.

Local land use planning has profound impacts on environmental quality; however, few empirical studies have been conducted to systematically measure local land use plans' environmental assessment quality and to identify the factors influencing it. This paper analyses the quality of 40 environmental impact reports (EIRs) of local jurisdictions' land use plans in California. A plan evaluation protocol defined by five core components and 63 indicators is developed to measure the quality of local land use plans' EIRs. The descriptive results indicate that the local jurisdictions produce relatively good quality on its EIRs, but there is still much room for improvement. There are large variations in the quality of EIRs across local jurisdictions. The regression results further highlight three major factors that can significantly influence local land use plan's EIR quality: number of planners, plan updating ability, and development pressure.

10/00422 Flooding of municipal solid waste landfills – an environmental hazard?

Laner, D. *et al. Science of the Total Environment*, 2009, 407, (12), 3674–3680.

Municipal solid waste (MSW) landfills pose a long-lasting risk for humans and the environment. While landfill emissions under regular operating conditions are well investigated, landfill behaviour and associated emissions in case of flooding are widely unknown, although damages have been documented. This paper aims at developing a methodology for determining the proportion of MSW landfills endangered by flooding, and at evaluating the impact flooded landfills might have on the environment during a flood event. The risk of flooding of MSW landfills is assessed by using information about flood risk zones. Out of 1064 landfills investigated in Austria, 312 sites or about 30% are located in or next to areas flooded on average once in 200 years. Around 5% of these landfills are equipped with flood protection facilities. Material inventories of 147 landfill sites endangered by flooding are established, and potential emissions during a flood event are estimated by assuming the worst case of complete landfill leaching and erosion. The environmental relevance of emissions during flooding is discussed on the basis of a case study in the western part of Austria. Although environmental hazards need to be assessed on a site- and event-specific basis, the results indicate that flooded MSW landfills represent in general small environmental risks for the period of flooding. The longer term consequences of flooding are discussed in a next paper.

10/00423 Global trading versus linking: architectures for international emissions trading

Flachsland, C. *et al. Energy Policy*, 2009, 37, (5), 1637–1647.

International emissions trading is widely seen as an indispensable policy pillar of climate change mitigation. This article analyses five different types of trading architectures, classified into two top–down (UNFCCC driven) and three bottom–up (driven by individual countries or regions) approaches. The two types of approaches are characterized by a trade-off between environmental effectiveness and political feasibility, respectively, whereas their relative cost-effectiveness depends on implementation details. Bottom–up architectures constitute imperfect substitutes for top–down architectures in terms of environmental effectiveness, and thus remain mere fallback options. However, especially the 'formal linking' architecture can act as complement in terms of cost-effectiveness.

10/00424 Hazard assessment of complex hydrides as hydrogen storage materials

Tanaka, H. *et al. International Journal of Hydrogen Energy*, 2009, 34, (7), 3210–3218.

Hydrogen storage materials containing $NaAlH_4$, $LiNH_2$, $Mg(NH_2)_2$, LiH and $LiBH_4$ were subjected to standardized safety tests in order to assess the potential hazards caused by the environmental exposure of these materials. All the materials were judged 'flammable', 'pyrophoric' and 'water-reactive', resulted in being classified as the United Nations Packing Group I, the most stringent category of container regulations in transporting these materials. A small spark energy (1.4 mJ) can trigger an intense dust cloud explosion of the $Mg(NH_2)_2 + LiH$ system of which the minimum explosive concentration was determined to be $90\,mg\,dm^{-3}$. Although this value is lower than those of the hydrogen storage alloys, the minimum explosive concentration of complex hydrides can be comparable to the alloys if expressed in terms of the amount of stored hydrogen in the material. Also examined was the eruption test, a non-standard test, in which the sample powder was pushed out of a container into the atmosphere by pressurized H_2. Despite the pyrophoricity, the authors observed only one explosion of the Ti-doped $NaAlH_4$ in dozens of trials using all the materials. A comparison with other materials points to the inevitability of more cautious measures than metal hydrides when handling these complex hydrides.

10/00425 Health effects of exposure to carbon nanofibers: systematic review, critical appraisal, meta analysis and research to practice perspectives

Genaidy, A. *et al. Science of the Total Environment*, 2009, 407, (12), 3686–3701.

Literature reviews examining the relationship between exposure to carbon nanofibres (CNFs) and health consequences are qualitative in nature and do not employ an evidence-based assessment. This research deals with a systematic review, critical appraisal, and meta-analysis designed to examine the potential health effects associated with exposure to CNFs. The utilization of research findings into practice is also explored. Twenty-one experimental studies satisfied the inclusion criteria and were performed on human cells, experimental animal models and animal cells as experimental units. The methodological qualities of published studies ranged from 'very poor' to 'excellent', with 'overall study description' scoring 'good' and 'study execution' equal to 'moderate'. The random-effects model was applied in the meta-analysis calculations as heterogeneity was significant at the 10% for all outcomes reported. The mean standardized meta-estimates for the experimental groups were significantly lower than those for the control groups for cell viability and cell death, respectively. Incorporating the effect of overall study quality score widened the gap between the experimental and control groups. Assessment of the research findings on the basis of the four-step algorithm revealed that the likelihood of the results to occur in practice is 'somewhat possible' at this time. That is, if exposure conditions to CNF in the reported studies are similar to those in nano-manufacturing plants, it is somewhat possible that CNFs alter the function of human cells resulting in loss of cell viability and cell death. Although the weight of evidence is not sufficient, it is advisable that actions be taken to ensure the protection of workers exposed to CNFs, that is, (a) engineering controls should be established to contain exposure to CNF, and (b) simultaneously rigorous personnel protective equipment should be planned to further minimize the risk of CNF exposure.

10/00426 Hydrochemical characteristics and seasonal influence on the pollution by acid mine drainage in the Odiel river Basin (SW Spain)

Sarmiento, A. M. *et al. Applied Geochemistry*, 2009, 24, (4), 697–714.
The Odiel river Basin is heavily affected by acid mine drainage (AMD) from the sulfide mining areas in the Iberian Pyrite Belt (IPB). A thorough study has been conducted along this fluvial system, monitoring the seasonal influence on the pollution level and its hydrochemical characteristics. From 2002 to 2006, surface water samples were collected at 91 different points throughout the Odiel river basin and analysed by field and laboratory methods for dissolved metals and metalloids. Acid mine drainage affects 37% of the length of the drainage network, which shows a great diversity of geochemical conditions as well as significant variations through the hydrological year. Unaffected streams show different water types depending on the lithological substrate and the marine aerosol influence. Mean concentrations in the contaminated streams are very high: 231 mg/L of Fe, 135 mg/L of Al, 56 mg/L of Zn, 16 mg/L of Cu, etc. Four types of contaminated streams were recognized based on hydrochemical and physicochemical characteristics. There are important seasonal variations depending on the precipitation regimen, level of pollution and proximity to the AMD sources. In the more contaminated samples the M/Fe ratio (M = metals other than Fe) decreases during the summer season. Slightly contaminated samples show an inverse evolution as this ratio increases in spring and summer due to substantial Fe precipitation. A recomparison of contaminant loads suggests that the Odiel river Basin (including the Tinto river) accounts for 15% of the global gross flux of dissolved Zn and 3% of the global gross flux of dissolved Cu transported by rivers into the ocean.

10/00427 Identifying sources of respirable quartz and silica dust in underground coal mines in southern West Virginia, western Virginia, and eastern Kentucky

Schatzel, S. J. *International Journal of Coal Geology*, 2009, 78, (2), 110–118.
Prior research has suggested that the source of respirable silica dust in underground coal mines is typically the immediate top or bottom lithology adjacent to the mined seam, not mineral matter bound within the mined coal bed. Geochemical analyses were applied in an effort to identify the specific source rock of respirable quartz dust in coal mines. The analyses also demonstrate the compositional changes that take place in the generation of the respirable dust fraction from parent rock material. All six mine sites were mining coal with relatively low mineral matter content, although two mines were operating in the Fire Clay coal bed which contains a persistent tonstein. Interpretations of Ca, Mg, Mn, Na, and K concentrations strongly suggest that the top strata above the mined seam is the primary source of mineral dust produced during mining. One site indicates a mixed or bottom source, possibly due to site specific conditions. Respirable dust compositional analyses suggest a direct relationship between the quantity of mineral Si and the quantity of quartz Si. A similar relationship was not found in either the top or bottom rocks adjacent to the mined seam. An apparent loss of elemental Al was noted in the respirable dust fraction when compared to potential parent rock sources. Elemental Al is present in top and bottom rock strata within illite, kaolinite, feldspar, and chlorite. A possible explanation for loss of Al in the respirable dust samples is the removal of clays and possibly chlorite minerals. It is expected that removal of this portion of the Al bearing mineral matter occurs during rock abrasion and dust transport prior to dust capture on the samplers.

10/00428 Informed and uninformed public opinions on CO_2 capture and storage technologies in the Netherlands

de Best-Waldhober, M. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (3), 322–332.
Two research methods were used in this study to analyse the awareness and perception of the Dutch general public regarding carbon dioxide capture and storage (CCS). In an information-choice questionnaire (ICQ), a representative sample of the Dutch public ($n = 995$) was provided with all information on attributes of six CCS options, which experts deemed necessary to come to well-considered and well-informed opinions. A traditional questionnaire was used simultaneously ($n = 327$) to study uninformed evaluations of these technologies. The results showed that the Dutch public is mostly unaware of CCS and has little knowledge about how current energy use causes global warming. Uninformed respondents are still inclined to give their opinion however, which results in unpredictive, easily changeable opinions. ICQ respondents who processed information on attributes of CCS options were likely to base their option evaluations on this information, though not entirely. All in all, the results of the ICQ suggest that, after processing information deemed necessary by experts, Dutch people reluctantly agree with large-scale implementation of each of the six CCS options.

10/00429 Land use change sector contribution to the carbon historical emissions and the sustainability – case study of the Brazilian Legal Amazon

de Araújo, M. S. M. *et al. Renewable and Sustainable Energy Reviews*, 2009, 13, (3), 696–702.
The paper presents five methodological aspects for the historic land use change accountability to compare two databases: the Historical Database on the Global Environment of RIVM, National Institute of Public Health and the Environment, adapted by the IVIG, International Virtual Institute of Global Change of the Federal University of Rio de Janeiro, named HYDE/IVIG and the Brazilian National Institute of Spatial Research database, named INPE database. The five aspects here considered are geographic limits; scale; basic methodology; deforestation concept; vegetal classification. It also presents their importance for the results of the calculus of deforested areas in the Brazilian Legal Amazon case. The use of the two databases information for carbon emissions calculation showed to be useful in terms of magnitude but not for qualitative analysis. The calculus of deforested areas is approximately similar for the period analysed. According to HYDE/IVIG, the Brazilian Legal Amazon land use changes representing agriculture and pasture lands, account 422,070 km^2, between 1750 and 1990 and the natural areas modified were originally classified as three types: tropical forest, wooded tropical forest and savanna. According to INPE, the cumulative Brazilian Legal Amazon deforestation until 1990 accounts 415,000 km^2 and the natural areas modified were originally classified as nine types. It means that different carbon contents by unit of deforestation have to be taken into account for the carbon emissions calculus. These numbers show the compatibility of the databases in terms of magnitude but the quality of the information present huge differences.

10/00430 Local air pollution and global climate change: a combined cost-benefit analysis

Bollen, J. *et al. Resource and Energy Economics*, 2009, 31, (3), 161–181.
This paper presents the findings of a combined cost-benefit analysis of local air pollution and global climate change, two subjects that are usually studied separately. Yet these distinct environmental problems are closely related, since they are both driven by the nature of present energy production and consumption patterns. The study demonstrates the mutual relevance of, and interaction between, policies designed to address these two environmental challenges individually. Given the many dimensions air pollution control and climate change management have in common, it is surprising that they have only little been analysed in combination so far. This study attempts to cover at least part of the existing gap in the literature by assessing how costs and benefits of technologies and strategies that jointly tackle these two environmental problems can best be balanced. By using specific technological options that cut down local air pollution, e.g. related to particulate emissions, one may concurrently reduce CO_2 emissions and thus contribute to diminishing global climate change. Inversely, some of the long-term climate change strategies simultaneously improve the quality of air in the short run. The well-established MERGE model has been extended by including emissions of particulate matter, and show that integrated environmental policies generate net global welfare benefits. The authors also demonstrate that the discounted benefits of local air pollution reduction significantly outweigh those of global climate change mitigation, at least by a factor of 2, but in most cases of the sensitivity analysis much more. Design policies are needed that simultaneously address the issues raised, as their combination creates an additional climate change bonus. As such, climate change mitigation proves an ancillary benefit of air pollution reduction, rather than the other way around.

10/00431 Management of plant health risks associated with processing of plant-based wastes: a review

Noble, R. *et al. Bioresource Technology*, 2009, 100, (14), 3431–3446.
The rise in international trade of plants and plant products has increased the risk of introduction and spread of plant pathogens and pests. In addition, new risks are arising from the implementation of more environmentally friendly methods of biodegradable waste disposal, such as composting and anaerobic digestion. As these disposal methods do not involve sterilization, there is good evidence that certain plant pathogens and pests can survive these processes. The

temperature/time profile of the disposal process is the most significant and easily defined factor in controlling plant pathogens and pests. In this review, the current evidence for temperature/time effects on plant pathogens and pests is summarized. The advantages and disadvantages of direct and indirect process validation for the verification of composting processes, to determine their efficacy in destroying plant pathogens and pests in biowaste, are discussed. The availability of detection technology and its appropriateness for assessing the survival of quarantine organisms is also reviewed.

10/00432 Model development for the estimation of fission product release under normal and accident conditions in a HTGR

Jeong, H. *et al. Nuclear Engineering and Design*, 2009, 239, (6), 1066–1075.

This article has attempted to estimate the radioactivity release from fuel materials during normal and transient conditions by coupling the TRISO fracture and the fission product (FP) diffusion. Two calculation models, named TRISO Fracture Analyser (TRIFA) and DIFfusion Analyser (DIFA), are developed. TRIFA is initially used to calculate the fraction of fractured fuel particles, thus determining the amount of fission gas release. The obtained particle fracture function is then used as input for the diffusion rate calculation. DIFA simulates with a single spherical fuel element, a pebble, irradiated under normal and accident conditions. It describes the diffusive transport of fission products by numerically solving the diffusion equation. The finite difference method is applied to obtain fission product release rates from a pebble to coolant. The model comparisons show that the new developed models are reliable, fast, and correspond with previous results of other models. As for HTR-10, the coupled models, TRIFA and DIFA, are applied to calculate the level of fission product release after accidents. The following conclusions can be drawn. First, the mitigation should be carried out until the maximum fuel temperature reaches under transient. Second, the mitigation should be intensively considered if the burn-up exceeds 5%FIMA (48 GWd/MTU) when transient happens. Additionally, it is found that there is the threshold burn-up where the rapid FP release occurs due to the numerous TRISOs fractured. Further investigations are needed to extend the use of the method developed in this work to the safety assessments for high-temperature gas-cooled reactors (HTGRs). This article will hopefully serve as a platform for designing the advanced TRISO that can minimize the activity release, and providing the rationale of development of the intensive accident mitigation system in future.

10/00433 Strategic environmental assessment as catalyst of healthier spatial planning: the Danish guidance and practice

Kørnøv, L. *Environmental Impact Assessment Review*, 2009, 29, (1), 60–65.

A wide range of factors within spatial planning can affect health. There is therefore an important scope for strategic environmental assessment (SEA) of spatial plans to protect and improve human health. Due to the EU Directive 2001/42/EC on SEA, health has been made explicit in Danish legislation and guidance. This paper examines the inclusion of health as a formal component in impact assessment of spatial plans. Based upon a documentary study of 100 environmental reports, the paper analyses and discusses how health impact considerations are incorporated in SEA practice. It is found that health impacts are included in SEA practice and are being interpreted in a broader sense than that exemplified by the national guidance. The frequently included health aspects are noise, drinking water, air pollution, recreation/outdoor life and traffic safety. The primary determinant for health is transport – whether it is at the overall or local planning level. The main conclusion is that SEA shows a potential to catalyse healthier spatial planning. Despite the broad inclusion of health in SEA practice the examination shows potential improvements, hereunder qualification of assessments by better explaining the nature and significance of impacts and by including the distributional aspects of human health impacts. Inclusion from the health sector is put forward as an important institutional mean to secure cross disciplinarily and higher quality assessment.

10/00434 The multi-annual carbon budget of a peat-covered catchment

Worrall, F. *et al. Science of the Total Environment*, 2009, 407, (13), 4084–4094.

This study estimates the complete carbon budget of an 11.4 km^2 peat-covered catchment in Northern England. The budget considers both fluvial and gaseous carbon fluxes and includes estimates of particulate organic carbon (POC); dissolved organic carbon (DOC); excess dissolved CO_2; release of methane (CH_4); net ecosystem respiration of CO_2; and uptake of CO_2 by primary productivity. All components except CH_4 were measured directly in the catchment and annual carbon budgets were calculated for the catchment between 1993 and 2005 using both extrapolation and interpolation methods. The study shows that over the 13 year study period the total carbon balance varied between a net sink of −20 to −91 Mg C/km^2/yr. The biggest component of this budget is the uptake of carbon by primary productivity (−178 Mg C/km^2/yr) and in most years the second largest component is the loss of DOC from the peat profile (+39 Mg C/km^2/yr). Direct exchanges of C with the atmosphere average −89 Mg C/km^2/yr in the catchment. Extrapolating the general findings of the carbon budget across all UK peatlands results in an approximate carbon balance of −1.2 Tg C/yr (±0.4 Pg C/yr) which is larger than previously reported values. Carbon budgets should always be reported with a clear statement of the techniques used and errors involved as this is significant when comparing results across studies.

CO_2, NO_x, SO_2 and particulate emissions

10/00435 An estimation of energy and GHG emission intensity caused by energy consumption in Korea: an energy IO approach

Chung, W.-S. *et al. Applied Energy*, 2009, 86, (10), 1902–1914.

In Korea, 97% of the energy resources are imported. The growth rate of greenhouse gas (GHG) emission per capita in the country was the highest in the world during 1990 and 2004. Moreover, 83% of the domestic GHG emissions stemmed from energy use in the year 2004. Therefore, there is an urgent need to develop an econometric model for energy intensity and GHG emission intensity in view of the poor energy endowment and environmental situation in Korea.In this study, a 96 × 96 hybrid energy input–output (E-IO) table was constructed by using energy units for each energy sector from the 2000 Korean IO table developed by the Bank of Korea in 2003. By using this E-IO table, the amount of energy intensities and GHG emission intensities, caused by energy use, were estimated for each sector. It was revealed that in the case of direct energy use, the average values of the direct energy intensity and GHG emission intensity of 96 economic sectors were 0.186 ton of oil equivalent (TOE)/million Korean Won (M-KRW) and 0.315 t-CO_2-eq./M-KRW, respectively. Further, in the case of total energy use, the average values of the total or embodied energy intensity and GHG emission intensity of these sectors were estimated to be 0.640 TOE/M-KRW and 1.534 t-CO_2-eq./M-KRW, respectively. From this integrated model, it is indicated that in order for Korea's energy and environment countermeasure not to slow down the economic activity as well as achieve GHG reduction, the GHG emission and energy use characteristics of whole sectors must be taken into consideration simultaneously.

10/00436 Analytical and experimental research for decreasing nitrogen oxides emissions

Jarquin-López, G. *et al. Applied Thermal Engineering*, 2009, 29, (8–9), 1614–1621.

This paper presents analytical as well as experimental research methods focused on decreasing nitrogen oxides formation while burning natural gas in a furnace of an 80 MW boiler. For this work different methods are investigated such as: the recirculation of smoke gases in the burners both in hot air and fuel; injection of water in the burning zone with the simultaneous decrease of the excess air coefficient into the burning zone including the organization of two stage burning in a furnace. The effects of combining these methods are investigated in order to obtain the maximum reduction in the concentration of nitrogen oxides exiting the burning zone. Operating modes of the boiler with the recirculation of smoke gases in hot air are used as a reference in calculating NO_x formation and NO_x emissions are measured from the stack of the boiler.

10/00437 Carbon dioxide ($C^{16}O_2$ and $C^{18}O_2$) absorption in zeolite Y materials: effect of cation, adsorbed water and particle size

Galhotra, P. *et al. Energy & Environmental Science*, 2009, (2), 401–409.

In this study, CO_2 adsorption in the presence and absence of co-adsorbed H_2O was investigated in zeolite Y. Several different zeolite Y materials were investigated including commercial NaY, commercial NaY ion-exchanged with Ba^{2+} and nanocrystalline NaY; herein referred to as NaY, BaY and nano-NaY. Following heating of these zeolites to 573 K and cooling to room temperature, CO_2 was adsorbed as a function of pressure. FTIR spectra show that a majority of CO_2 adsorbs in the pores of these three zeolites (NaY, BaY and nano-NaY) in a linear complex with the exchangeable cation, as indicated by the intense absorption band near 2350 cm^{-1}, assigned to the ν_3 asymmetric stretch of adsorbed CO_2. Most interestingly is the formation of carbonate and bicarbonate on the external surface of nano-NaY zeolites as indicated by the presence of several broad absorption bands in the 1200–1800 cm^{-1} region, suggesting unique sites for CO_2

adsorption on the surface of the nanomaterial. For the other two zeolite materials investigated, bicarbonate formation is only evident in BaY zeolite in the presence of co-adsorbed water. Adsorption of ^{18}O-labelled carbon dioxide and theoretical quantum chemical calculations confirm these assignments and conclusions.

10/00438 Carbon sequestration in coal-beds with structural deformation effects

Liu, G. and Smirnov, A. V. *Energy Conversion and Management*, 2009, 50, (6), 1586–1594.

Carbon dioxide sequestration in a coal-bed is a profitable method to reduce the concentration of greenhouse gas in the atmosphere and to recover byproduct methane from the coal seam. The important factor to be considered is the stability of the coal-bed with the increased carbon dioxide injection. It is crucial to avoid carbon dioxide escaping from the coal seam caused by structural deformation. Meanwhile, structural deformation also depends on such properties of the geological coal basin as fracture state and phase equilibrium, especially the porosity, permeability and saturation of the coal seam. In this study, a structural deformation effect was simulated with the purpose of predicting carbon dioxide storage in the environment of a typical unmineable coal seam. As an example, the Appalachian Basin is considered in the deformation analysis of carbon dioxide sequestration based on the variable saturation model. Moreover, the comparison between simulations with and without the account of structural deformation is given. The results indicate that modelling of structural deformation in carbon sequestration is feasible by directly coupling structure terms to a variable saturated model. Moreover, introducing structural deformation effects into carbon sequestration modelling is important because it affects the fluid flow and leads to a faster drop of the resulting capillary pressure and relative permeability of the gas phase. This faster drop directly results in the diminished carbon dioxide storage capacity in a coal-bed basin. In addition, structural deformation modelling in carbon sequestration simulations can provide important insights into how to avoid carbon leakage and seepage by monitoring the effective stress and displacement of coal-bed basin during carbon dioxide injection.

10/00439 Carbonic anhydrase-facilitated CO_2 absorption with polyacrylamide buffering bead capture

Dilmore, R. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (4), 401–410.

A novel CO_2 separation concept is described wherein the enzyme carbonic anhydrase (CA) is used to increase the overall rate of CO_2 absorption after which hydrated CO_2 reacts with regenerable amine-bearing polyacrylamide buffering beads (PABB). Following saturation of the material's immobilized tertiary amines, CA-bearing carrier water is separated and recycled to the absorption stage while CO_2-loaded material is thermally regenerated. Process application of this concept would involve operation of two or more columns in parallel with thermal regeneration with low-pressure steam taking place after the capacity of a column of amine-bearing polymeric material was exceeded. PABB CO_2-bearing capacity was evaluated by thermogravimetric analysis (TGA) for beads of three acrylamido buffering monomer ingredient concentrations: 0 mol/kg bead, 0.857 mol/kg bead, and 2 mol/kg bead. TGA results demonstrate that CO_2-bearing capacity increases with increasing PABB buffering concentration and that up to 78% of the theoretical CO_2-bearing capacity was realized in prepared PABB samples (0.857 mol/kg recipe). The highest observed CO_2-bearing capacity of PABB was 1.37 mol of CO_2 per kg dry bead. TGA was also used to assess the regenerability of CO_2-loaded PABB. Preliminary results suggest that CO_2 is partially driven from PABB samples at temperatures as low as 55 °C, with complete regeneration occurring at 100 °C. Other physical characteristics of PABB are discussed. In addition, the effectiveness of bovine carbonic anhydrase for the catalysis of CO_2 dissolution is evaluated. Potential benefits and drawbacks of the proposed process are discussed.

10/00440 Characterization of flue gas desulfurization particulates in equalization basins

Iannacone, M. M. *et al. Fuel*, 2009, 88, (9), 1580–1587.

Particulates in pilot-scale flue gas desulfurization (FGD) scrubber water were characterized by powder X-ray diffraction, scanning electron microscopy with energy dispersive spectroscopy, and size analysis based on Stokes' Law after settling in an equalization basin of a pilot-scale constructed wetland treatment system. Three sources were interpreted for specific particle types identified in samples analysed: FGD wet scrubbing processes, coal combustion byproducts, and uncombusted material from coal. Gypsum ($CaSO_4 \cdot 2H_2O$) from the FGD scrubbing process comprises ~95% of the particulates. Iron oxide particles and cenospheres in the particulate samples are interpreted as coal combustion products. Particles interpreted as originating from unburned coal contain carbon and metals including Zn and Fe. The most abundant elements in the particulates analysed are O, C, Ca, S, Fe, and Si, with maximum mean content of individual elements ranging from 13% to 70% among particle types. Less abundant elements include Al, K, Mg, Ti, and Mo, with maximum mean content from 0.1% to 3.8%.

10/00441 Combining GTL fuel, reformed EGR and HC-SCR aftertreatment system to reduce diesel NO_x emissions. A statistical approach

Rodríguez-Fernández, J. *et al. International Journal of Hydrogen Energy*, 2009, 34, (6), 2789–2799.

An ultra-low sulfur diesel (ULSD) fuel and a synthetic gas-to-liquid (GTL) fuel, besides different types of standard and reformed exhaust gas recirculation (EGR), were evaluated in a single-cylinder, direct injection, diesel engine equipped with hydrocarbon-selective catalytic reduction (HC-SCR) aftertreatment system. The results obtained were statistically analysed (at 95% statistical significance) to identify the most significant factors that affect NO_x emissions and to search for the optimum operation conditions in order to minimize these emissions. For that purpose, a fully crossed factorial experimental design was used, including two different engine speeds (1200 and 1500 rpm), two engine loads (25% and 50%), and four EGR/REGR ratios (0%, 10%, 20% and 30%) resulting in almost one hundred tests. An optimal combination of fuel type, REGR type and REGR ratio was proved to reduce around 89–95% of the reference NO_x emissions. In general, at 25% engine load GTL fuelling combined with the reformed EGR with the highest hydrogen content was found the most desirable, as the hydrogen sharply increased the NO_x conversion in the SCR catalyst. Differently, at 50% load standard EGR was sufficient to reach high NO_x reductions. These findings may be used for the implementation of a system on-board capable to switch from EGR to REGR, which will help engine manufacturers to meet the future emission regulations.

10/00442 Experimental study on mercury transformation and removal in coal-fired boiler flue gases

Wang, Y. *et al. Fuel Processing Technology*, 2009, 90, (5), 643–651.

This paper reports mercury speciation and emissions from five coal-fired power stations in China. The standard Ontario Hydro Method (OHM) was used into the flue gas mercury sampling before and after fabric filter (FF)/electrostatic precipitator (ESP) locations in these coal-fired power stations, and then various mercury speciation such as Hg^0, Hg^{2+} and Hg^P in flue gas, was analysed by using the EPA method. The solid samples such as coal, bottom ash and ESP ash, were analysed by DMA 80 based on EPA Method 7473. Through analysis the mercury speciation varied greatly when flue gas went through FF/ESP. Of the total mercury in flue gas, the concentration of Hg^{2+} is in the range of 0.11–14.76 μg/N m^3 before FF/ESP and 0.02–21.20 μg/N m^3 after FF/ESP; the concentration of Hg^0 ranges in 1.18–33.63 μg/N m^3 before FF/ESP and 0.77–13.57 μg/N m^3 after FF/ESP, and that of Hg^P is in the scope of 0–12.11 μg/N m^3 before FF/ESP and 0–0.54 μg/N m^3 after FF/ESP. The proportion of Hg^{2+} ranges from 4.87%–50.93% before FF/ESP and 2.02%–75.55% after FF/ESP, while that of Hg^0 is between 13.81%–94.79% before FF/ESP and 15.69%–98% after FF/ESP, with that of Hg^P is in the range of 0%–45.13% before FF/ESP and 0%–11.03% after FF/ESP. The mercury in flue gas mainly existed in the forms of Hg^0 and Hg^{2+}. The concentrations of chlorine and sulfur in coal and flue gas influence the species of Hg that are formed in the flue gas entering air pollution control devices. The concentrations of chlorine, sulfur and mercury in coal and the compositions of fly ash had significant effects on mercury emissions.

10/00443 Greenhouse gas emissions from low-temperature oxidation and spontaneous combustion at open-cut coal mines in Australia

Carras, J. N. *et al. International Journal of Coal Geology*, 2009, 78, (2), 161–168.

Spontaneous combustion and low-temperature oxidation of waste coal in open-cut coal mines represents a potentially large source of greenhouse gas emissions. In this paper, emission fluxes of CO_2 and CH_4 from spoil piles and waste coal dumps measured at 11 mines in the Hunter Valley and Bowen Basin in Australia are presented. The data displayed considerable scatter, which is consistent with the inhomogeneous nature of spoil pile material and permeability of surfaces. Despite the scatter, emissions were able to be classified into three broad categories according to the intensity of the spontaneous combustion present in the material. Average emissions ranged from about 12 kg CO_2-e yr^{-1} m^2 to 8200 kg CO_2-e yr^{-1} m^{-2}, depending on the intensity of the spontaneous combustion. There was also, within the scatter of the data, an approximately linear trend of increasing emission flux with increasing surface temperature. A key finding of the research is that the emission rates of greenhouse gases from spoil piles where there is no spontaneous combustion, but only low-temperature oxidation of coal and coal waste, are similar to the emission rates due to biological activity from vegetated surfaces. However, further research is required to quantify the degree to which spoil piles that have no spontaneous combustion contribute to the anthropogenic atmospheric CO_2 burden.

10/00444 Low-energy sodium hydroxide recovery for CO_2 capture from atmospheric air – thermodynamic analysis

Mahmoudkhani, M. and Keith, D. W. *International Journal of Greenhouse Gas Control*, 2009, 3, (4), 376–384.

To reduce the risks of climate change, atmospheric concentrations of greenhouse gases must be lowered. Direct capture of CO_2 from ambient air, 'air capture', might be one of the few methods capable of systematically managing dispersed emissions. The most commonly proposed method for air capture is a wet scrubbing technique which absorbs CO_2 in an alkaline absorbent, i.e. sodium hydroxide producing an aqueous solution of sodium hydroxide and sodium carbonate. In most of the previous works it was assumed that the absorbent would be regenerated and CO_2 liberated from the alkaline carbonate solution using a lime and calcium carbonate causticization cycle. The authors describe a novel technique for recovering sodium hydroxide from an aqueous alkaline solution of sodium carbonate and present an end-to-end energy and exergy analysis. In the first step of the recovery process, anhydrous sodium carbonate is separated from the concentrated sodium hydroxide solution using a two-step precipitation and crystallization process. The anhydrous sodium carbonate is then causticized using sodium tri-titanate. The titanate direct causticization process has been of interest for the pulp and paper industry and has been tested at lab- and pilot-scale. In the causticization process, sodium hydroxide is regenerated and carbon dioxide is liberated as a pure stream, which is compressed for use or disposal. The technique requires 50% less high-grade heat than conventional causticization and the maximum temperature required is reduced by at least 50 °C. This titanate cycle may allow a substantial reduction in the overall cost of direct air capture.

10/00445 NO emission on pulverized coal combustion in high temperature air from circulating fluidized bed – an experimental study

Zhu, J. *et al. Fuel Processing Technology*, 2009, 90, (5), 664–670.

High temperature air was adopted by combustion in high excess air ratio in a circulating fluidized bed. Experiments on pulverized coal combustion in high temperature air from the circulating fluidized bed were carried out in a down-fired combustor with the diameter of 220 mm and the height of 3000 mm. The NO emission decreases with increasing the residence time of pulverized coal in the reducing zone, and the NO emission increases with excess air ratio, furnace temperature, coal mean size and oxygen concentration in high temperature air. The results also revealed that the co-existing of air-staging combustion with high temperature air is very effective to reduce nitrogen oxide emission for pulverized coal combustion in the down-fired combustor.

10/00446 Pathways for conversion of char nitrogen to nitric oxide during pulverized coal combustion

Molina, A. *et al. Combustion and Flame*, 2009, 156, (3), 574–587.

The conversion of nitrogen in char (char-N) to NO was studied both experimentally and computationally. In the experiments, pulverized coal char was produced from a US high-volatile bituminous coal and burned in a dilute suspension at 1170 K, 1370 K and 1570 K, at an excess oxygen concentration of 8% (dry), with different levels of background NO. In some experiments, hydrogen bromide (HBr) was added to the vitiated air as a tool to alter the concentration of gas-phase radicals. During char combustion, low NO concentration and high temperature promoted the conversion of char-N to NO. HBr addition altered NO production in a way that depended on temperature. At 1170 K the presence of HBr increased NO production by 80%, whereas the addition of HBr decreased NO production at higher temperatures by 20%. To explain these results, three mechanistic descriptions of char-N evolution during combustion were evaluated with computational models that simulated (a) homogeneous chemistry in a plug-flow reactor with entrained particle combustion, and (b) homogeneous chemistry in the boundary layer surrounding a reacting particle. The observed effect of HBr on NO production could only be captured by a chemical mechanism that considered significant release of HCN from the char particle. Release of HCN also explained changes in NO production with temperature and NO concentration. Thus, the combination of experiments and simulations suggests that HCN evolution from the char during pulverized coal combustion plays an essential role in net NO production.

10/00447 The acceptability of CO_2 capture and storage (CCS) in Europe: an assessment of the key determining factors: part 1. Scientific, technical and economic dimensions

de Coninck, H. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (3), 333–343.

The ACCSEPT project, which ran from January 2006 to December 2007, identified and analysed the main factors which have been influencing the emergence of CO_2 capture and geological storage (CCS) within the European Union (EU). The key clusters of factors concern science and technology, law and regulation, economics, and social acceptance. These factors have been analysed through interviews, a large-scale questionnaire conducted in 2006, and discussions in two stakeholder workshops (2006 and 2007). Part I of this paper aims to distil the key messages and findings with regards to scientific, technical, legal and economic issues. There are no compelling scientific, technical, legal, or economic reasons why CCS could not be widely deployed in the forthcoming decades as part of a package of climate change mitigation options. In order to facilitate this deployment, governments at both the EU and Member State levels have an important role to play, in particular in establishing a robust and transparent legal framework (e.g. governing long-term environmental liability) and a strong policy framework providing sufficient and long-term incentives for CCS and CO_2 transportation networks.

10/00448 The acceptability of CO_2 capture and storage (CCS) in Europe: an assessment of the key determining factors: part 2. The social acceptability of CCS and the wider impacts and repercussions of its implementation

Shackley, S. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (3), 344–356.

Part 1 of this study presented the findings of the EU ACCSEPT project (2006–2007) with regards to scientific, technical, legal and economic issues. Part 2 presents the analysis of social acceptability on the part of both the lay public and stakeholders. The authors examine the acceptability of CO_2 capture and geological storage (CCS) within the Clean Development Mechanism (CDM) of the Kyoto Protocol. The debate over the inclusion of CCS within the CDM is caught-up in a set of complex debates that are partly technical and partly political and, therefore, difficult, and time-consuming, to resolve. The study explores concerns that support for CCS will detract from support for other low-carbon energy sources, although no evidence was found that support for CCS is currently detracting from support for renewable energy sources, though it is probably too early to detect such an effect. Efforts at understanding, engaging with, and communicating to, the lay public and wider stakeholder community (not just business) in Europe are currently weak and inadequate, despite well-meaning statements from governments and industry.

10/00449 The use of guide to the expression of uncertainty in measurement for uncertainty management in National Greenhouse Gas Inventories

Velychko, O. and Gordiyenko, T. *International Journal of Greenhouse Gas Control*, 2009, 3, (4), 514–517.

Significant attention is paid to common questions relative to the methods of the expression of the uncertainty of measurements and the estimates of the results of the definition of the environmental characteristics of global objects. Peculiarities of the expression of uncertainty and the variants of its estimation in international metrological and environmental guides are shown. Basic positions concerning the uncertainty estimates of obtained results, shown in well-known international guides of inventory of GHG, are considered. Metrological and environmental guide's comparison has shown peculiarities of used terms and uncertainty analysis with correlation and covariance of input values. Environmental guides use more simplified but specific approaches of the uncertainty analysis. Specific approaches to estimation of the uncertainty in trend of GHG emissions imply realization of long-term observation and also environmental guide's consideration correlation of data across years. The algorithm of expressing uncertainty and scheme for estimating uncertainty according to environmental guides are proposed. It is necessary to apply a well-known international metrological guide, which is developed by international organizations in the field metrology, standardization, physicists and chemistry, during the preparation of environmental guides concerning the analysis of uncertainty. The use of international metrological guidance of expression of measurements uncertainty in development of new and reconsideration of old international environmental guides is recommended.

Hydrocarbon emissions

10/00450 A statistical approach to develop a detailed soot growth model using PAH characteristics

Raj, A. *et al. Combustion and Flame*, 2009, 156, (4), 896–913.

The model used in this study describes the structure and growth of planar PAH molecules, and is referred to as the kinetic Monte Carlo–aromatic site (KMC-ARS) model. A detailed PAH growth mechanism based on reactions at radical sites available in the literature, and additional reactions obtained from quantum chemistry calculations are used to model the PAH growth processes. New rates for the reactions involved in the cyclodehydrogenation process for the formation of six-member rings on PAHs are calculated based on density functional theory simulations. The KMC-ARS model is validated by comparing experimentally observed ensembles on PAHs with the computed ensembles for a C_2H_2 and a C_6H_6 flame at different heights above the burner. This lays the groundwork for a detailed soot particle population balance model which describes the evolution of an ensemble of soot particles based on their PAH structure. However, at present incorporating such a detailed model into a population balance is computationally unfeasible. Therefore, a simpler model referred to as the site-counting model has been developed, which replaces the structural information of the PAH molecules by their functional groups augmented with statistical closure expressions. This closure is obtained from the KMC-ARS model, which is used to develop correlations and statistics in different flame environments which describe such PAH structural information. These correlations and statistics are implemented in the site-counting model, and results from the site-counting model and the KMC-ARS model are in good agreement. Additionally the effect of steric hindrance in large PAH structures is investigated and correlations for sites unavailable for reaction are presented.

10/00451 Concentrations, sources, and spatial distribution of individual polycyclic aromatic hydrocarbons (PAHs) in agricultural soils in the Eastern part of the EU: Poland as a case study

Maliszewska-Kordybach, B. *et al. Science of the Total Environment*, 2009, 407, (12), 3746–3753.

Soils from agricultural areas receive unsatisfactory attention as regards the contamination with organic pollutants. To answer those needs the contents of the 16 individual polycyclic aromatic hydrocarbon compounds were determined (GC/MS technique) in agricultural soils in Poland. The samples ($n = 216$) were collected from the upper layer of arable land in the year 2005. Half of the samples represented typical rural areas, while the rest derived from the territories potentially subjected to the urban/industrial pressure of various intensity. The mean (geometric) content of individual compounds varied from $1\,\mu g\,kg^{-1}$ for acenaphtylene to $55\,\mu g\,kg^{-1}$ for fluoranthene with the highest contributions (11.6%–12.9%) of phenanthrene, fluoranthene and pyrene. Higher molecular weight PAHs (four rings) were strongly linked mutually and with the $\Sigma 16$ PAHs. They contributed substantially (73%) to the overall content of PAHs, which implies domination of anthropogenic sources. The calculated molecular indexes suggest that most of those PAHs derive from the combustion of coal, the main energy source in Poland. Simultaneously, the concentrations of lower molecular weight compounds seem to reflect the background, 'natural' PAH compounds, which represent mainly atmospherically distributed emission. The division of the samples into groups describing geographical regions and landscape type enabled evaluation of the spatial trends in contamination of soils with PAH compounds. The most pronounced effect of spatial parameters corresponded to PAHs of more than four rings, while lower molecular weight compounds showed more homogeneous concentration through the country.

10/00452 Improved sectoral allocation of NMVOC emissions from solvent use in Greece

Sidiropoulos, C. and Tsilingiridis, G. *Science of the Total Environment*, 2009, 407, (13), 4075–4083.

Solvent use and road transport are the two most significant sources of non-methane volatile organic compound (NMVOC) emissions in urban environments. The allocation of emissions to solvent-related activities is of major importance since it is a major step towards providing spatially and temporally resolved accurate emission data in air quality models and assisting the development of properly orientated emission reduction measures. In this paper an activity-specific NMVOC emission inventory from solvent use in Greece is presented. The diversity, the volume and the complexity of the relevant activity data and, in some cases, the use of the same solvent and/or product in a variety of uses are the main difficulties in solvent emission inventorying. To overcome them, an extensive market research/survey is performed, combined with a literature review and expert opinion, to determine solvent utilization factors (expressed via usage factors as solvents, or per activity and/or per process). With the aid of these usage factors, appropriate emission factors, national statistical activity data and the calculating formulas developed, emissions are estimated and attributed to each solvent-related activity. Main results indicate that the use of solvents is the second source of NMVOC emissions in Greece (72 ± 4 kt in 2003), the road transport sector being the first one (171 kt). Paint applications are the most important source of solvent NMVOC emissions, accounting for $44.5 \pm 2.5\%$ of the total solvent NMVOC followed by the domestic use of solvents (excluding paint), which accounts for $39 \pm 2\%$ of total solvent NMVOC.

16 ENERGY

Supplies, policy, economics, forecasts

10/00453 California's renewables portfolio standard: charting the course towards 33% by 2020

Wong Kup, J. *et al. The Electricity Journal*, 2009, 22, (4), 79–94.

California contributes approximately 1.8% of the total global, and 7.5% of the United States, greenhouse gas (GHG) emissions. The Global Warming Solutions Act of 2006, Assembly Bill (AB) 32, requires California to reduce its GHG emissions to 1990 levels by 2020. Meeting this target will require cutting approximately 30% from business-as-usual emission levels projected for 2020, or about 15% from today's levels. Although the latest figures show that a number of contracted renewable projects are beginning to deliver, much improvement is still needed for California to stay on track to reach 33% by 2020. Beyond the long-recognized transmission infrastructure and permitting barriers, the current credit crisis has made renewable development even more challenging. The Stimulus Act provides substantial assistance and encouragement, but it still may not be enough to continue driving the market absent wider economic recovery. Nonetheless, as University of California at Berkeley, Energy and Resources Professor Daniel Kammen recently commented, 'the pipeline is rich'. Thus, a 33% RPS by 2020 is now realistically within reach.

10/00454 Certification framework based on effective trapping for geologic carbon sequestration

Oldenburg, C. M. *et al. International Journal of Greenhouse Gas Control*, 2009, 3, (4), 444–457.

In this study a certification framework (CF) was developed for certifying the safety and effectiveness of geologic carbon sequestration (GCS) sites. Safety and effectiveness are achieved if CO_2 and displaced brine have no significant impact on humans, other living things, resources, or the environment. In the CF, effective trapping was related to CO_2 leakage risk which takes into account both the impact and probability of leakage. The authors achieve simplicity in the CF by using (1) wells and faults as the potential leakage pathways, (2) compartments to represent environmental resources that may be impacted by leakage, (3) CO_2 fluxes and concentrations in the compartments as proxies for impact to vulnerable entities, (4) broad ranges of storage formation properties to generate a catalogue of simulated plume movements, and (5) probabilities of intersection of the CO_2 plume with the conduits and compartments. The approach was demonstrated on a hypothetical GCS site in a Texas Gulf Coast saline formation. Through its generality and flexibility, the CF can contribute to the assessment of risk of CO_2 and brine leakage as part of the certification process for licensing and permitting of GCS sites around the world regardless of the specific regulations in place in any given country.

10/00455 Divestitures in the electricity sector: conceptual issues and lessons from international experiences

Weight, H. *et al. The Electricity Journal*, 2009, 22, (3), 57–69.

Competition policy is an important tool of governments to establish functioning markets, particularly in the scope of liberalizing the energy sector. An examination of horizontal divestitures in several markets suggests that in appropriate cases divestiture can enhance competition in the electricity sector.

10/00456 Potential energy demand for cooling in the 50 largest metropolitan areas of the world: implications for developing countries

Sivak, M. *Energy Policy*, 2009, 37, (4), 1382–1384.

Air conditioning of dwellings in developing countries is currently rather rare, but increasing personal income is expected to change that. This study examined the potential energy demand for cooling in the 50 most populous metropolitan areas of the world, and assessed the incremental demand in developing countries that this would create on top of the current energy demand due to heating. The analysis used local cooling and heating degree-day data. The main results are as follows: (1) Most of the largest metropolitan areas are in developing countries (38 out of 50), and most of them, in turn, are in warm to hot climates. (2) All but two of the top 30 metropolitan areas in terms of cooling degree days are in developing countries. (3) The potential cooling demands are greater than heating demands in most of the metropolitan areas that are in developing countries (24 out of 38). The main implication of these findings is that increasing personal income is likely to lead to an unprecedented increase in energy demand in many developing countries. For example, the potential cooling demand in metropolitan Mumbai is about 24% of the demand for the entire United States.

10/00457 Strategic partitioning of emission allowances under the EU Emission Trading Scheme

Böhringer, C. and Rosendahl, K. E. *Resource and Energy Economics*, 2009, 31, (3), 182–197.

The EU Emission Trading Scheme (ETS) is breaking new ground in the experience with emission trading regimes across multiple jurisdictions. Since the EU ETS covers only some industries, it implies a hybrid emission control scheme where EU member states must apply complementary domestic emissions regulation for the non-trading sectors of their economies in order to comply with their national emission reduction targets. The EU ETS thus opens up for strategic partitioning of national emissions budgets by the member states between trading and non-trading sectors. In this paper, the potential effects of such strategic behaviour on compliance cost and emissions prices is examined. It is shown that concerns on efficiency losses from strategic partitioning are misplaced. In turn, the analysis implicitly indicates significant political economy forces behind EU climate policy, as both cost-effective and strategically motivated partitioning of national emission budgets are far off from the actual break-down between trading and non-trading sectors.

10/00458 Sustainable energy planning by using multi-criteria analysis application in the island of Crete

Tsoutsos, T. *et al. Energy Policy*, 2009, 37, (5), 1587–1600.

The sustainable energy planning includes a variety of objectives, as the decision-making is directly related to the processes of analysis and management of different types of information (technological, environmental, economic and social). Very often, the traditional evaluation methods, such as the cost-benefit analysis and macro-economic indicators, are not sufficient to integrate all the elements included in an environmentally thorough energy plan. On the contrary the multiple criteria methods provide a tool, which is more appropriate to assemble and to handle a wide range of variables that is evaluated in different ways and thus offer valid decision support. This paper exploits the multi-criteria methodology for the sustainable energy planning on the island of Crete in Greece. A set of energy planning alternatives are determined upon the implementation of installations of renewable energy sources on the island and are assessed against economic, technical, social and environmental criteria identified by the actors involved in the energy planning arena. The study constitutes an exploratory analysis with the potential to assist decision makers responsible for regional energy planning, providing them the possibility of creating classifications of alternative sustainable energy alternatives.

10/00459 Taking 'control': Federal energy regulatory commission policy on acquisitions of electric utility securities

Bloom, D. I. and O'Brien, A. D. *The Electricity Journal*, 2009, 22, (4), 43–52.

Section 203 of the Federal Power Act remains subject to considerable uncertainty. Therefore, it is important to keep several rules in mind. Each potential acquisition must be separately analysed under Section 203(a)(1) and 203(a)(2) of the Act. A proposed acquisition that is exempt or preapproved under one provision may still require prior FERC approval under the other one.

10/00460 The energy-GDP nexus: evidence from a panel of Pacific Island countries

Mishra, V. *et al. Resource and Energy Economics*, 2009, 31, (3), 210–220.

The Pacific Island countries are small island economies that are increasingly dependent on energy for growth and development, yet highly susceptible to climate change. Thus, the relationship between energy consumption and GDP is crucial for realizing their future development and growth objectives. This article tests for Granger causality and provides long-run structural estimates for the relationship between energy consumption, GDP and urbanization for a panel of Pacific Island countries. For the panel as a whole in the long-run there is bidirectional Granger causality between energy consumption and GDP and these variables exert a positive impact on each other. A 1% increase in energy consumption increases GDP by 0.11%, while a 1% increase in GDP increases energy consumption by 0.23%. The findings suggest that for the panel as a whole these countries should increase investment in energy infrastructure and regulatory reform of energy infrastructure to improve delivery efficiency, continue to promote alternative energy sources and put in place energy conservation policies to reduce unnecessary wastage. These strategies seek to realize the dual objectives of reducing the adverse effects of energy use on the environment, while avoiding the negative effect on economic growth of reducing energy consumption.

10/00461 Towards cooperative policy approaches in China – drivers for voluntary agreements on industrial energy efficiency in Nanjing

Eichhorst, U. and Bongardt, D. *Energy Policy*, 2009, 37, (5), 1855–1865.

Energy efficiency is a national priority for China as rapid energy consumption growth aggravates its greenhouse gas emissions, local air pollution and energy scarcity. In the 1990s, a large number of voluntary agreements emerged in industrialized countries in order to improve industrial energy efficiency. These experiences are now taken into account in China. This article analyses the drivers for voluntary agreements on industrial energy efficiency in China, based on a case study of three enterprises in Nanjing, Jiangsu Province. Furthermore, the article reviews the institutional set-up of energy policy and investigates the pertaining policy culture. From the findings, conclusions are drawn on the role of voluntary agreements within China's larger policy context. It is concluded that opposed to avoiding stricter regulation, voluntary agreements in Nanjing are reinterpreted in view of more stringent national provisions on energy efficiency in the 11th Five Year Plan. Hence, agreements have evolved into an implementation tool of national policy at the local level. For industry, another major driver for participation was identified as improving its relations with local authorities. Voluntary agreements showed to have the potential to overcome traditional constraints of implementing top–down policies at the local level in China.

10/00462 Voluntary agreements with white certificates for energy efficiency improvement as a hybrid policy instrument

Oikonomou, V. *et al. Energy Policy*, 2009, 37, (5), 1970–1982.

In this paper, the authors examine the implementation of a combined policy scheme that consists of a traditional instrument, the voluntary agreements, and an innovative one, the white certificates. The basic structure of this scheme is that energy suppliers who undertake an energy efficiency obligation under a white certificate scheme can make use of voluntary actions to enhance investments in innovative energy savings projects. Energy suppliers and other market parties can additionally or in parallel participate in voluntary agreements and set energy efficiency targets. For fulfilling their voluntary agreement target, these market parties can receive tax exemptions or receive white certificates that they can sell in the market. Transaction costs and baseline definition for demonstrating energy efficiency improvement deserve special attention. This policy can assist a country to enhance energy efficiency improvement while it stimulates innovation. Cost effectiveness can be higher than the case of stand-alone policy instruments, since more financing options are available for more expensive projects. Nevertheless, the added value of the scheme lies more in the implementation of innovative measures for enhanced energy efficiency. Furthermore, market parties can discover more business opportunities in energy efficiency and establish a green image; hence an integrated scheme should achieve higher political acceptability.

Energy conservation

10/00463 Comparison of energy conservation building codes of Iran, Turkey, Germany, China, ISO 9164 and EN 832

Fayaz, R. and Kari, B. M. *Applied Energy*, 2009, 86, (10), 1949–1955.

To improve the energy efficiency of buildings via compliance to regulation in Iran, Code No. 19 was devised in 1991. The code lacks high-level aims and objectives, addressing the characteristics of Iranian buildings. As a consequence, the code has been revised and is not completely implemented in practice, and still remains inefficient. As with any energy coding system, this code has to identify the right balance between the different energy variables for the Iranian climate and way of life. In order to assist improvements to high-level objectives of Code 19, this code is compared with ISO 9164, EN 832, German regulation, TS 825 of Turkey and China's GB 50189 to understand how these have adapted international standards to national features. In order to test the appropriateness of Code 19, five case study buildings in Iran are assessed against Code 19 as well as Turkish standard TS 825 and the results are compared. The results demonstrate that Code 19 is efficient in calculations of building envelope, but it needs improvements in the areas of ventilation, gains from internal and solar sources. The paper offers suggestions for improving the code.

10/00464 Corporate social responsibility for implementation of sustainable energy development in Baltic States

Streimikiene, D. *et al. Renewable and Sustainable Energy Reviews*, 2009, 13, (4), 813–824.

This article analyses the main problems and challenges of corporate social responsibility in energy sector in Baltic States. Development of socially responsible business in energy sector can provide for the implementation of sustainable energy development without state interventions. This voluntary measure implemented by energy enterprises can ensure efficient public–private partnership in achieving sustainable development targets. The analysis of corporate social responsibility development in energy sector of Baltic States is provided and positive impact of corporate social responsibility on sustainable energy development is evaluated.

10/00465 Distributed generation and trigeneration: energy saving opportunities in Italian supermarket sector

Arteconi, A. *et al. Applied Thermal Engineering*, 2009, 29, (8–9), 1735–1743.

This paper presents an analysis of the potential for introducing distributed generation systems in the supermarket sector in the light of Italian legislation (inasmuch as concerns tax incentives and regulations) with a view to arriving at some generally applicable criteria. The energy users in question are characterized by a strong demand for energy for refrigeration for food preservation and for ambient air-conditioning during the summer. This makes supermarkets particularly suitable for trigeneration applications with the prime mover coupled with absorption systems. This study analyses the feasibility of implementing trigeneration systems for the combined production of electricity and ambient heating and air-conditioning energy or, alternatively, for the combined generation of electrical energy and refrigeration for the preservation of food. Finally, the hypothesis of combining trigeneration systems with photovoltaic systems aimed at maximizing the energy saving achievable was also considered. This paper analyses the various technologies from a technical, economic and environmental standpoint, enabling advantages and disadvantages to be identified in relation to a real case.

10/00466 Introducing a new model for material savings in the Finnish paper industry

Lodenius, M. *et al. Resources, Conservation and Recycling*, 2009, 53, (5), 255–261.

The paper industry is one of major material and energy users in Finland, material costs being far bigger than energy costs. Energy saving is promoted in Finland by an energy service centre, subsidies and energy service companies (ESCOs). Material savings in production processes are typically used to reduce costs while life-cycle material efficiency would require more focus, e.g. on product design, which could be promoted by total producer responsibility, economic instruments and environmental permits. For industrial sites with limited resources, MASCOs' (Material Saving Companies) services could manage material savings, e.g. by funding the investments, planning and running the project. Authorities should put more emphasis on material auditing and information on material saving technologies and logistics. Material savings should also be included into the environmental permitting procedures. Materials saving services are developing and the projected Finnish material efficiency service centre could support new businesses. This article is based on a literature review and interviews of persons in paper producing companies and environmental authorities. Experiences of the first MASCO project in Finland are also analysed.

10/00467 Modelling and analysis of air-cooled reciprocating chiller and demand energy savings using passive cooling

Chowdhury, A. A. *et al. Applied Thermal Engineering*, 2009, 29, (8–9), 1825–1830.

The study presents modelling and analysis of air-cooled chiller system in an office building at Central Queensland University in Rockhampton, Australia. EnergyPlus, building energy simulation software, has been used to model and to simulate the energy savings. Base case cooling energy has been compared with measured data. The simulated results show a reasonable agreement with the measured data. As a passive cooling means, the effect of economizer usages and pre-cooling have been simulated and analysed to assess annual demand savings for an energy intensive office building at Rockhampton, Australia. It was found that implementation of the pre-cooling and economizer system could save 115 kW/m^2/month and 72 kW/m^2/month total cooling energy and 26 kW/m^2/month and 42 kW/m^2/month chiller energy, respectively.

10/00468 Polygeneration and efficient use of natural resources

Serra, L. M. *et al. Energy*, 2009, 34, (5), 575–586.

The consumption of natural resources has been increasing continuously during recent decades, due to the growing demand caused by both the economic and the demographic rise of global population. Environmental overloads that endanger the survival of our civilization and the sustainability of current life support systems are caused by the increased consumption of natural resources – particularly water and energy – which are essential for life and for the socio-economic development of societies. While not yet well utilized, process integration and polygeneration are promising tools that reach the double objective of increasing the efficiency of natural resources, and also minimizing the environmental impact. This paper discusses the concepts of polygeneration and energy integration and various examples of polygeneration systems: (i) sugar and energy production in a sugarcane factory; (ii) district heating and cooling with natural gas cogeneration engines and (iii) combined production of water and energy. It is clearly evident that polygeneration systems which include appropriate process integration significantly increase the efficient use of natural resources.

10/00469 Quantification of the impact of the end-of-life scenario on the overall resource consumption for a dwelling house

Dewulf, J. *et al. Resources, Conservation and Recycling*, 2009, 53, (4), 231–236.

In this work, fractions that are the result of the demolition phase of a dwelling house have been investigated with respect to their recovery potential: stony material, wood, metals, glass, synthetic materials and a rest fraction. Depending on their nature, different alternative end-of-life scenarios have been investigated to replace disposal, such as re-use, recycling or incineration with heat and electricity production. All resources necessary for these scenarios have been inventoried. At the same time, those that are not longer necessary for the disposal and those that would have been necessary to make the obtained products from virgin resources are quantified. Based on these three items, the overall balance results into the calculation of net virgin resource savings for different end-of-life scenarios, quantified in cumulative exergy consumption (MJ of exergy). For this specific case, the best end-of-life scenario can save virgin natural resources with a content of 258 GJ of exergy. Looking at the entire life cycle of the house, i.e. construction phase, use phase and end-of-life phase, the quantitative analysis shows a saving of virgin natural resources of 15% with the implementation of the best end-of-life scenario instead of disposal as end-of-life.

10/00470 Sustainable energy options for Pakistan

Asif, M. *et al. Renewable and Sustainable Energy Reviews*, 2009, 13, (4), 903–909.

With the advent of the year 2008, Pakistan faces a gap of 4500 MW between the demand and supply of electricity, registering a shortfall of 40%. The article provides an overview of the key dimensions of the crisis, i.e. growing gap between demand and supply, diminishing indigenous oil and gas reserves, rising energy cost and security concerns. It also explores hydropower, solar energy, biomass and wind power as sustainable energy options for the country. In has been found that the total estimated hydropower potential is more than 42 GW out of which only 6.5 GW has been tapped so far. In terms of available solar energy Pakistan is amongst the richest countries in the world, having an annual global irradiance value of 1900–2200 kWh/m^2. Despite that fact that the biomass plays an important role in the primary energy mix by contributing to 36% of the total supplies, it has not managed to break into the commercial energy market. Wind power, also been identified as a potential source of energy, is yet to take off.

10/00471 The impact of the daylight saving time on electricity consumption – a case study from Jordan

Momani, M. A. *et al. Energy Policy*, 2009, 37, (5), 2042–2051.

The paper examines the impact of daylight saving time (DST) on electricity consumption in Jordan. Two types of analysis were done: the first analysis examines the impact of DST on the lighting loads based on a survey study made for residential and commercial sectors. The second examines the impact of DST on the over all electricity generation through analysing the daily load curves (DLCs) before and after the DST onset and removal in 2000 and 2007. The results show that the application of DST during the year 2000 saves the electricity used for illumination by –0.73% but it increases the overall generation at the onset and removal of DST by 0.5% and 1.4% due to increase in the heating and cooling loads. The analysis of DLCs during the year 2007 shows similar effects as in the year 2000 except during the early morning period at the DST onset where DST decreases the demand during this time. The analysis shows that DST decreases the electricity demand at DST onset by 0.2% and increases it at DST removal by 0.3%. A possible decrease in the electricity consumption may take place if the DST is implemented from April to end of August.

17 ENERGY CONVERSION AND RECYCLING

10/00472 Biohydrogen production from biomass and industrial wastes by dark fermentation

Chong, M.-L. *et al. International Journal of Hydrogen Energy*, 2009, 34, (8), 3277–3287.

Hydrogen is a clean energy carrier which has a great potential to be an alternative fuel. Abundant biomass from various industries could be a source for biohydrogen production where combination of waste treatment and energy production would be an advantage. This article summarizes the dark fermentative biohydrogen production from biomass. Types of potential biomass that could be the source for biohydrogen generation such as food and starch-based wastes, cellulosic materials, dairy wastes, palm oil mill effluent and glycerol are discussed in this article. Moreover, the microorganisms, factors affecting biohydrogen production such as undissociated acid, hydrogen partial pressure and metal ions are also discussed.

10/00473 Electrochemical performance of a hybrid direct carbon fuel cell powered by pyrolysed MDF

Jain, S. L. *et al. Energy Environmental Science*, 2009, 2, (6), 687–693.

Medium density fibreboard is a ubiquitous element in modern furniture, this study considers utilizing waste MDF as a future energy source. In particular, the authors focus upon the hybrid direct carbon fuel cell (HDCFC), which involves a combined molten carbonate/solid oxide fuel cell anode/electrolyte interface and can be fuelled by a wide range of carbon forms. Current–voltage measurements and a.c. impedance at temperatures in the range of 525–800 °C have been made on cells powered by pyrolysed medium density fibreboard (pMDF) samples which had undergone three different preparatory treatments (immersion of strips in molten eutectic carbonate mixture; deep soaking of strips in aqueous carbonate mixture corresponding to the eutectic composition and fine powdering). Below 700 °C the three pMDF samples show quite different electrochemical performance in the HDCFC, but above 700 °C their behaviour becomes similar. Powdered pMDF gives the best OCV (0.89 V) and lowest resistance (2.36 Ω) values below 700 °C, although the electrochemical performance is dominated by diffusion limitations and the performance degrades at higher temperatures. The immersed strip behaves quite differently with limited performance below 750 °C but it shows both good OCV, 1 V, and low resistance, <4 Ω, at higher temperatures. Three components are discernable, an ohmic contribution probably due to both ionic resistance of zirconia electrolyte and electronic resistance of current collection and two electrode processes thought to be associated with the transfer of oxygen ions at the electrode/electrolyte interface and diffusion of reactant species through the electrode. The activation energies calculated from the ohmic resistances for the three samples (−0.79 to −1.00 eV) are of similar order to that expected for the yttria zirconia electrolyte.

10/00474 Experimental study of exhaust-gas energy recycling efficiency of hybrid pneumatic power system

Huang, K. D. *et al. International Journal of Energy Research*, 2009, 33, (10), 931–942.

A hybrid pneumatic power system (HPPS) comprises an internal combustion engine (ICE), an air compressor, a high-pressure air storage tank, and a turbine, which stores the flow work instead of a battery's electrochemical energy; moreover, this system can recycle the exhaust-gas energy and make the ICE operate at its optimal point. Therefore, it can be viewed as a promising solution to increase a system's thermal efficiency and greatly improving exhaust emissions. This paper presents experimental study results concerning the operating capabilities of the HPPS and the effect of the contraction of the cross-sectional area (CSA) at the merging region of the energy merger pipe for the change in the compressed airflow pressure (P_{air}) on the exhaust-gas energy recycling of the HPPS. The experiments were performed on an HPPS that uses an innovative energy merger pipe with a total length of 530 mm, a diameter of 34 mm, and an angle between the two pipes of 30°, and the CSA was adjusted for the change in P_{air}. The experimental results show that the exhaust-gas energy recycling and the merger flow energy are significantly dependent on the CSA adjustment for the change in P_{air}. The optimum conditions for the best merging process can be achieved at a CSA of around 5–35% in the full range of P_{air}. Under these conditions, the exhaust-gas energy recycling efficiency reached approximately 75–81%; therefore, a vehicle equipped with an HPPS can achieve efficiency that is approximately 40% higher than that of conventional vehicles.

10/00475 Jet flames of a refuse derived fuel

Weber, R. *et al. Combustion and Flame*, 2009, 156, (4), 922–927.

This paper is concerned with combustion of a refuse derived fuel in a small-scale flame. The objective is to provide a direct comparison of the RDF flame properties with properties of pulverized coal flames fired under similar boundary conditions. Measurements of temperature, gas composition (O_2, CO_2, CO, NO) and burnout have demonstrated fundamental differences between the coal flames and the RDF flames. The pulverized coals ignite in the close vicinity of the burner and most of the combustion is completed within the first 300 ms. Despite the high volatile content of the RDF, its combustion extends far into the furnace and after 1.8 s residence time only a 94% burnout has been achieved. This effect has been attributed not only to the larger particle size of fluffy RDF particles but also to differences in RDF volatiles if compared to coal volatiles. Substantial amounts of oily tars have been observed in the RDF flames even though the flame temperatures exceeded 1300 °C. The presence of these tars has enhanced the slagging propensity of RDF flames and rapidly growing deposits of high carbon content have been observed.

10/00476 Parametric analysis of heat and mass transfer regenerators using a generalized effectiveness-NTU method

Sphaier, L. A. *et al. International Journal of Heat and Mass Transfer*, 2009, 52, (9–10), 2265–2272.

A parametric analysis of heat and mass transfer in regenerative exchangers that employ sorbent materials has been performed. The adopted methodology is based on the effectiveness-NTU (number of transfer units) approach, traditionally employed for analysing sensible heat exchangers. However, a generalization was developed to account for the effects of coupled heat and mass transfer, matrix diffusion, as well as physical adsorption. The generalized approach was applied to a unified mathematical formulation for this class of exchangers and the potential of the methodology was demonstrated through an analysis of the influence of several dimensionless parameters on regenerator performance.

10/00477 Pyrolysis of mixed plastics for the recovery of useful products

Siddiqui, M. N. and Redhwi, H. H. *Fuel Processing Technology*, 2009, 90, (4), 545–552.

Thermal and catalytic pyrolysis of polystyrene (PS) with low-density polyethylene (LDPE), high-density polyethylene (HDPE), polypropylene (PP), poly-ethylene terephthalate (PET) plastics were carried out in a 25 cm^3 stainless steel micro reactor at around 430–440 °C under 5.5–6.0 MPa of N_2 gas pressure for 1 h. Three reactions of each plastic with PS were conducted in the ratio of 1:1, 1:2 and 1:3. The amount of PS was varied to explore its role and reactivity. In all coprocessing reactions, ratio 1:1 afforded the best yields in the form pyrolytic oils. Simulated distillation of hexane soluble portion showed that the low boiling fractions were not found and fractions were obtained only after 96 °C + boiling point. It could be due to the vaporization of high volatile components. In most of the binary pyrolysis, light cycle oil (LCO) fractions have low recovery than heavy cycle oil (HCO). GC identified some very important chemical compounds present in the liquid products obtained from the pyrolysis of mixed plastics. The results obtained from this study have shown usefulness and feasibility of the pyrolysis process of the mixed plastics as an alternative approach to feedstock recycling.

10/00478 Transesterification of soybean frying oil to biodiesel using heterogeneous catalysts

Georgogianni, K. G. *et al. Fuel Processing Technology*, 2009, 90, (5), 671–676.

The present work studied the transesterification reaction of soybean frying oil with methanol, in the presence of different heterogeneous catalysts (Mg MCM-41, Mg-Al Hydrotalcite, and K^+ impregnated zirconia), using low frequency ultrasonication (24 KHz) and mechanical stirring (600 rpm) for the production of biodiesel fuel. Selection of catalysts was based on a combination of porosity and surface basicity. Their characterization was carried out using X-ray diffraction, nitrogen adsorption-desorption porosimetry and scanning electron microscopy (SEM) with energy dispersive spectra (EDS). The activities of the catalysts were related to their basic strength. Mg-Al hydrotalcite in particular showed the highest activity (conversion 97%). It is important to mention that the catalyst activity of ZrO_2 in the transesterification reaction increased as the catalyst was enriched with more potassium cations becoming more basic. Use of ultrasonication significantly accelerated the transesterification reaction compared to the use of mechanical stirring (5 h versus 24 h).

10/00479 Tri-potassium phosphate as a solid catalyst for biodiesel production from waste cooking oil

Guan, G. *et al. Fuel Processing Technology*, 2009, 90, (4), 520–524.

Transesterification of waste cooking oil with methanol, using tri-potassium phosphate as a solid catalyst, was investigated. Tri-potassium phosphate shows high catalytic properties for the transesterification reaction, compared to CaO and tri-sodium phosphate. Transesterification of waste cooking oil required approximately two times more solid catalyst than transesterification of sunflower oil. The fatty acid methyl ester (FAME) yield reached 97.3% when the transesterification was performed with a catalyst concentration of 4 wt% at 60 °C for 120 min. After regeneration of the used catalyst with aqueous KOH solution, the FAME yield recovered to 88%. Addition of a co-solvent changed the reaction state from three-phase to two-phase, but reduced the FAME yield, contrary to the results with homogeneous catalysts. The catalyst particles were easily agglomerated by the glycerol drops derived from the homogeneous liquid in the presence of co-solvents, reducing the catalytic activity.